

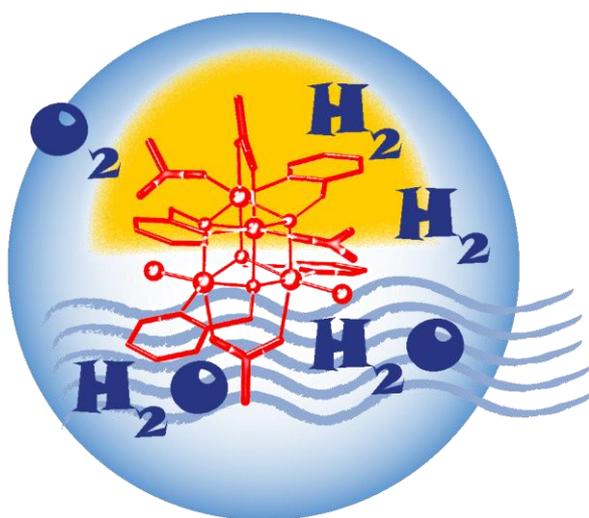


University of
Zurich^{UZH}

URPP LightChEC

Progress Report 2021

URPP LightChEC - Solar Light to Chemical Energy Conversion



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1 Management Summary

The ongoing global pandemic continued to impair the progress in LightChEC albeit to a lesser extent than in the previous year. A focus of the year 2021 was furthermore the move of most of the LightChEC members to the new lab space on the UZH Irchel Campus. The move caused further delay but came with the reward of now working in very good laboratories and being equipped with renewed and/or additional instrumentation.

Progress was still made along all directions according to the updated objectives of the last report. The concept of dual-core catalysts was pursued in the Alberto group. Two Co_2 and Ru_2 -based catalysts were thoroughly studied in all directions, the latter one for CO_2 reduction in particular. It was shown that some selected mononuclear Co-containing catalysts perform well in CO_2 reduction and not only in H_2 formation. We are evaluating photosensitizers with improved long-term stabilities and photochemical properties. Studies by the Patzke group brought forward a core step to the fabrication of manganese-oxide-based OECs, which showed long-term stability at constant current while being easily available via economically attractive routes. Fundamental progress was made in the debate on molecular vs. heterogeneous photocatalysts with a study that revealed the superior behavior of self-optimized cobalt-oxyhydroxides over molecular Co-catalysts and the structural prerequisites for their high OER performance. The Hamm group successfully started a new direction in CO_2 reduction, which may complement corresponding research in the Alberto group. Different materials layered on the surface with Ga_2O_3 , Ni or h-BN, as well as Sb_2S_3 in collaboration with the Tilley group are a focus of the Osterwalder group for understanding carrier separation dynamics. The important semiconductor system Sb_2Se_3 is the focus of the Tilley group along with various photo- and electrocatalytic aspects. In collaboration with the Alberto and the Osterwalder groups, molybdenum clusters were grafted on Sb_2Se_3 and electrocatalysis studied with (AP)XPS at PSI before and after the catalytic process. The theoretical and computational studies of the Hutter and Luber groups were conducted in close collaboration with the respective experimentalists. The Hutter group strongly involved machine learning for the OER whereas the Luber group supported the HER side with calculations of redox potentials. In terms of analytical progress, magneto-optical probing of metal-hydride forming electrodes as well as the conversion of ethylene to higher alkanes was successfully continued. Scientific progress on fundamental aspects of all kinds of light induced reactions or electrocatalysis was thus made in all directions. In addition, first attempts towards upscaling of catalyst materials were made (Patzke) and some contacts with companies were initiated (Alberto).

Even though most presentations and conferences took place online, networking was extended mainly towards PSI and Empa. One of the few exceptions was the live/virtual LightChEC symposium, which was hosted by Empa and raised interest beyond the LightChEC community. Importantly, especially for networking among the young researchers, the LightChEC discussion meeting did continue in a hybrid form. Attendance was good throughout. Additional individual collaborations were established outside UZH, mirroring the interest of external groups in our published achievements.

Finances were well balanced by the end of the year and no urgent additional needs with respect to instrumentation were submitted. The budget, although reduced by 50% for the last period, did not reduce the activities of the URPP substantially. This is due to constantly available additional funds but also due to students being supported from the respective regular budgets, a compelling case that LightChEC is now strongly established at UZH and the associated institutes. By the end of 2021 and the first year of the third period, the head of the URPP changed and Prof. Patzke will lead the URPP for the remaining period.

Another insight from the reporting year that already emerged in the preceding years is that the fruitful science of LightChEC should be complemented in the future with more intense outreach activities,

especially towards organizations which are active in the broader sustainable energy business or with overarching academic institutions. To start, for example, Prof. Patzke contributed a section on "Artificial Photosynthesis" as an emerging technology to the widely received and consulted 2021 Technology Outlook of the Swiss Academy of Technical Sciences (SATW).

2 Objectives

2.1 Objectives for the Reporting Year

2.1.1 Photocatalytic Water Reduction: WRCs and Photosensitizers (Prof. R. Alberto)

Water / CO₂ Reduction Catalysts

- Coupling two bis-bipyridyl moieties via different heterocycles into novel dual-core water reduction catalysts. Elucidating the mechanisms and performance with different electrochemical techniques. Profound electro- and photocatalysis since these are our best-performing WRCs.
- Derivatizing the cyclic porphyrin-based WRCs with groups different from phosphonates for embedding them into membranes or grafting them on sulfide or selenide materials (Tilley group).
- Benchmarking of polymerised vs monomeric WRCs in homogenous photocatalysis.
- Achieving a fully organic polymer-based photocathode (with Empa).
- Assessing the performance of [Mo₃S₄]⁴⁺ WRCs coordinated to tridentate ligands and comprising a heterometal "M", i.e. [Mo₃M'(L³)₃S₄]⁴⁺.

Photosensitizers

- Synthesis, physico-chemical studies of new water soluble photosensitizers with the core-cluster type [M₆E₈], e.g. [Re₆S₈]Br₆.
- Graft best catalysts on the new semiconductors for preparing photocathodes.

2.1.2 Visible-Light-Driven Water Oxidation Catalysts (WOCs) (Prof. G. R. Patzke)

In situ electrochemical TEM and XAS studies on perovskite-based OER electrocatalysts

We will investigate perovskite-type OER materials with outstanding electrochemical performance metrics and d-block metal cations other than Co (such as Mn or Fe) with the goal to substitute this relatively expensive metal component. For an in-depth understanding of their transformation under operational conditions, which is crucial for their efficient design in the first place, we will focus on the advanced combination of in situ electrochemical TEM investigations with operando XAS studies. With this knowledge at hand, we will also explore their corresponding HER activity for overall water splitting (e.g. through combination of perovskites and MoS₂ along the lines of our chalcogenide catalyst research).

Dynamic behaviour of spinel oxides and their structural evolution under OER conditions

Starting from our insight into the complex preparation-performance relations of spinel-type OERs, we will explore them parallel to the target perovskites with in situ electrochemical TEM and XAS techniques. Recent studies point to interesting operando dynamics of 3D transition metal spinel OER catalysts, which have been far less investigated than their perovskite counterparts have.

Long-term and large-scale performance of low cost manganese materials

To round off our investigations on an application-oriented note, we will aim to push the limits on manganese-based oxide OERs as representative materials for low cost technologies. Further mechanistic studies on our recently developed MnO_x electrodes with our operando repertoire will create a feedback loop for the optimization of their coating procedures to significantly scale up their production dimensions (e.g. with convenient spray coating or thermal decomposition routes). This will promote the sought-after synchronization of mechanistic understanding and efficient production of oxide catalysts for water splitting.

2.1.3 Time-resolved Spectroscopy of Artificial Photosynthetic Systems (Prof. P. Hamm)

- Observe transient intermediates in molecular CO₂ reduction systems.
- Continue towards a working hydrogen evolution system with a photosensitizer and a hydrogen evolution catalyst on an electron-donating semiconductor, such as NiO.
- Solvation of metal hydrides.

2.1.4 Surfaces (Prof. J. Osterwalder)

- Finishing the gallium oxide on Cu₂O(111) project and publish the results.
- Deposition of nickel metal on Fe₃O₄(001) surfaces to study the transition from a nickel single atom catalyst to the formation of a nickel ferrite surface.
- Preparation of hexagonal boron nitride layers on Cu(111) and Cu₂O surfaces and study of photoinduced charge dynamics in these systems.

2.1.5 Molecular Approaches to Renewable Energies (Prof. D. Tilley)

- Sb₂Se₃: Elucidation of the origin of the photovoltage improvement by ammonium sulfide etching and CuCl₂ treatment. Investigations with anchored molecular catalysts.
- Impedance spectroscopy: Now that we have a realistic model and know how to analyze impedance spectra of multi-layer photocathodes, we will use this technique to identify problematic layers and the effect of certain treatments towards improving device performance.
- Immobilization of molecular catalysts via host-guest interactions: we will continue our work in this new area with new hosts (e.g. cucurbiturils) and new anchoring moieties for the guests (e.g. amino coumarin) that enable a control of the binding strength via pH.

2.1.6 Computational Studies of Dynamic Properties of Water Oxidation (Prof. J. Hutter)

- We are going to extend the generation of machine learning potentials for other water-metal interfaces, considering, for instance, Ni, Pd, Cu, Ag, and Au. Moreover, we aim at introducing nuclear quantum effects, implementing specific training of path-integral trajectories.
- Using ab initio molecular dynamics simulations, we will study reaction processes among molecules adsorbed at oxide interfaces. The conditions of electrified interface can be taken into account in DFT simulations by applying external electric fields or exploiting ad-hoc designed surface functionalization and periodic boundary conditions.
- We still aim at the simulation of the dynamics of molecules at the interface under the influence of time-dependent fields. The focus is on the application of excited state dynamics, which has been successfully applied in literature to study light-induced processes of aqueous metallic nanoparticles.
- We will further investigate the hBN/Cu₂O system. The adsorption of metal atoms and metal clusters will be considered also as intercalated between the oxide and the overlayer. In this respect, we will focus on the formation of the oxygen vacancies, on possible reactive processes and on the effects on these latter of confinement at the interface.

2.1.7 Surfaces / H₂ and CO₂ Storage and Conversion (Prof. K.-H. Ernst)

- Creation of 2D MOFs on thin insulating films, such as MgO on Ag(100).
- Set-up of vacuum preparation / electrochemistry cell for testing of catalytic activity of MOFs.

- Creation of 2D MOFs with pentagonal symmetry.
- Creation of squarate-MOFs on HOPG.

2.1.8 Electronic Structure of Materials for Solar-Water Splitting (Dr. A. Borgschulte)

- Continuation of solar water splitting probed by magneto-optics with focus on metal hydride forming electrodes.
- Photoemission studies on hydrogenation of hydrogen evolution reaction electrodes using the hydrogen membrane approach focus on V, ZrV₂.
- Continuation of hydrogenation of gaseous organic compounds with focus on selective conversion ethylene to specific liquid alkanes (jet fuel).

2.1.9 Theoretical Chemistry (Prof. S. Luber)

- Continuation of the study of molecular Co-based water reduction catalysts on surfaces.
- Study of the redox potentials for mono- and dinuclear Co-based complexes in collaboration with experimentalists.
- Development of an approach for excited state dynamics of condensed phase systems.

2.2 Achieved Objectives and Milestones

2.2.1 Photocatalytic Water Reduction: WRCs and Photosensitizers (Prof. R. Alberto)

Water / CO₂ Reduction Catalysts

We coupled two bis-bipyridyl units via different heterocycles to yield dual-core catalysts. We have two examples in hand and investigated the photocatalytic H₂ formation efficiencies as a function of acid type, pH and other physico-chemical parameters (objective 1). We found that rates and TONs are not dramatically enhanced but the overpotential is reduced. Synthetic challenges slowed progress down (paper in preparation). No progress has been made on the grafting of pyrphrines but this work is currently resumed (objective 2). A large variety of polymerized WRCs has been synthesized and grafted on electrodes. They exhibited long-term electrochemical stabilities and efficient electrocatalytic H₂ formation. These cathodes are superior to homogeneous photocatalysis, albeit they cannot directly be compared (objective 3). The fully organic, polymer-based photocathode was prepared but was found to be not efficient enough to warrant further studies (objective 4). We synthesized different atom-precise molybdenum clusters based on Mo₃ cores and grafted them on Sb₂Se₃ semiconductors (with Tilley). Extensive XPS analytics before and after electrocatalysis are currently being evaluated but they show slow decomposition of the clusters (objective 5). Since we aim at going to heterogeneous systems, the photocatalytic activities in homogeneous solutions are not pursued for the moment.

Photosensitizers

We concentrated the search for new, long-term stable photosensitizers on octahedral rhenium clusters of the type {Re₆S₈}. Various clusters have been prepared by high temperature synthesis and they were fully characterized (objective 6). They showed very long excited-state life times and an extremely rapid oxidative quenching as required for photocatalysis. Catalytic systems are currently being explored. These clusters could not yet be grafted on surfaces due to the move into the new buildings (objective 7) but are ongoing for this year.

In collaboration with a German company, we prepared full water splitting cells. This collaboration is going on but it has been slowed down for Covid reasons.

2.2.2 Visible-Light-Driven Water Oxidation Catalysts (WOCs) (Prof. G. R. Patzke)

In situ electrochemical TEM and XAS studies on perovskite-based OER electrocatalysts

The studies on $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSM) as OER electrocatalysts by Esmael Balaghi pointed to a self-repair mechanism of the catalyst via the formation of a birnessite-type phase at the electrode interface. However, the preliminary X-ray absorption spectroscopy (XAS) data and X-ray pair distribution function analyses (PDF) concerning the characterization of the amorphous layer and of the species involved in the WOC reconstruction process need further refinement for publication.

Dynamic behaviour of spinel oxides and their structural evolution under OER conditions

Concerning the role of cobalt spinel oxides and related phases as OER photocatalysts (Lukas Reith), we finalized and published a comprehensive comparison of molecular Co-WOCs and disordered/amorphous Co-oxide phases in 2021 [26]. Extensive XAS investigations (with Dr. Carlos Triana) of different highly active Co-salt precipitates as WOCs (up to 91% photocatalytic oxygen yield) clearly revealed that optimal photocatalytic OER performance depends on a trade-off between at least three parameters. Generating optimal WOCs from straightforward Co-precursors requires a "sweet spot" regarding the crystal structure, the degree of crystallinity and the amount of Co(III) centers in the catalyst. We identified CoOOH as the most active WOC phase, in close relation to previous electrochemical studies, while the formation of Co_3O_4 spinel significantly decreased the overall OER activity.

Long-term and large-scale performance of low cost manganese materials

Our studies on the economic fabrication of manganese oxide-based catalysts (Dr. Sima Heidari) from thermal decomposition of low-cost KMnO_4 solutions were finally concluded and published in 2021 [14]. The high OER performance (> 100 h of stable current density of 1.0 mA/cm² at an overpotential of 490 mV under neutral conditions) compares favourably to related MnO_x catalysts and does not lead to any post-catalytic changes. The convenient (300 °C) and basically recyclable synthetic route is technologically attractive. Interestingly, in situ TEM monitoring revealed that the observed structural transformation routes of the manganese precursor depend on the analytical measurement conditions to a large extent.

2.2.3 Time-resolved Spectroscopy of Artificial Photosynthetic Systems (Prof. P. Hamm)

- Regarding CO_2 reduction, we obtained first results and a manuscript is in preparation, see discussion below.
- Regarding hydrogen evolution system on an electron-donating semiconductor surface, unfortunately, no progress has been made. We will stop this line of research.
- Regarding solvation of metal hydrides, a measurement series on a large variety of solvents exists and a manuscript is in preparation, see discussion below.

2.2.4 Surfaces (Prof. J. Osterwalder)

- Attempts to grow a coherent, well ordered interface of Ga_2O_3 on $\text{Cu}_2\text{O}(111)$ were continued. Annealing gallium oxide films grown with different thickness showed pronounced interdiffusion before crystalline order in the film could be established. Interestingly, the onset temperature of

diffusion was found to be higher in films grown on the reduced $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstructed cuprous oxide surface.

- Monolayer amounts of Ni metal were deposited on the $(\sqrt{2}\times\sqrt{2})R45^\circ$ reconstructed $\text{Fe}_3\text{O}_4(001)$ surface. Annealing studies of these films showed diffusion of Ni atoms into the subsurface starting at 250°C , occupying predominantly octahedral sites in the third atomic layer below the surface. This finding is consistent with the formation of a Ni-ferrite like phase.
- Hexagonal boron nitride (h-BN) monolayers were grown on Cu(111) surfaces. Exposure to oxygen pressures around 1 mbar led to the intercalation of oxygen between the h-BN layer and the metal surface. Annealing to 150°C induced the formation of a cuprous oxide like phase underneath the intact h-BN. layer. Photoexcited charge transfer dynamics will be studied in 2022.
- In addition, the charge carrier dynamics in $\text{Sb}_2\text{S}_3(110)$ was studied with time-resolved two-photon photoemission. A recently proposed scenario of self-trapping of free charge carriers via optical phonons was confirmed and a self-trapping time of 0.7 ps was determined.

2.2.5 Molecular Approaches to Renewable Energies (Prof. D. Tilley)

- Sb_2Se_3 : all points achieved. A manuscript regarding the ammonium sulfide and CuCl_2 treatment is in preparation. Molecular catalysts from the Alberto group were assessed on our thin films. The results were promising, but this project was put on the backburner to prioritize other projects.
- Impedance spectroscopy: achieved. Our published paper generated a lot of interest, and new collaborators in France sent us some samples for us to characterize with our new methodology.
- Immobilization of molecular catalysts via host-guest interactions: our previous plans were not fully achieved because we decided to pursue a new direction on this front: we newly purchased a quartz crystal microbalance (QCMB) and we investigated binding of the host-guest complexes by virtue of a mass change. It has not been straightforward, but we made good progress.

2.2.6 Computational Studies of Dynamic Properties of Water Oxidation (Prof. J. Hutter)

- We extended the generation of machine learning potentials for metal-water interfaces and now we have a library of potentials including Pt, Ni, Pd, Cu, Ag, Au for both the most common low index surfaces, i.e., (111) and (100).
- We refined the study on oxygen vacancies in Cu_2O , considering both bulk sites and surface sites. We could demonstrate that the formation of an oxygen vacancy is accompanied by the presence of polarons, preferably localized close to the surface, and it is expected to affect the electron mobility.
- We also considered additional models of cuprous oxide.
- We further investigated the competitive adsorption of formate and water at the titania surface. With the help of molecular dynamics and enhanced sampling we characterized the desorption/adsorption processes depending on coverage and temperature and determine the underlying free energy surface.

2.2.7 Surfaces / H_2 and CO_2 Storage and Conversion (Prof. K.-H. Ernst)

- Not achieved: Creation of 2D MOFs on thin insulating films, such as MgO on Ag(100) Because of the negative results on HOPG (see below) these experiments were postponed.
- Not achieved: Set-up vacuum preparation/electrochemistry cell for testing of catalytic activity of MOFs Because of the most likely rather destructive nature of electrochemical studies on MOFs, we have

decided not to continue this route of research. Instead, we have ordered iso-tope-labeled CO and CO₂ to study the adsorption/desorption and coordination/activation using FTIR spectroscopy, TDS and time-of-flight secondary ion mass spectrometry (ToF-SIMS). Despite ordering of the gasses early in 2021, delivery is scheduled by 11th of February 2022.

– Not achieved: Creation of 2D MOFs with pentagonal geometry

We have tried to prepare MOFs using Ni and pentagonal croconic acid on Au(111). STM shows a disordered layer and no regular MOF structure.

– Partly achieved: Creation of squarate-MOFs on HOPG

We have tried to prepared MOFs on HOPG and confirmed their formation using XPS. However, STM imaging was inconclusive. The problem is most likely the high mobility at low coverage and 3D island formation at higher coverage. We will instead focus on graphene/Ru(0001) where the adsorbates should be less decoupled and stabilized by the moiré structure.

Alternative approach taken: Determination of 3d/4f electronic structure and magnetism

Because we could not advance much in the proposed objectives, we focused on the determination of the 3d/4f electronic states of the metal atoms using XAS/XLD/XMCD. These results are important to rationalize potential catalytic properties by ab-initio theory. Four days of 24h beamtime at the XTreme beamline of SLS at PSI were performed in September 2021. We could determine the electronic structure of Ni, Co and Er-based MOFs on Au(111) (see section 3). In particular, the high-spin state of the Ni(II) ions is surprising and may be explained with a non-planar coordination-sphere.

2.2.8 Electronic Structure of Materials for Solar-Water Splitting (Dr. A. Borgschulte)

– Continuation of solar water splitting probed by magneto-optics with focus on metal hydride forming electrodes – not achieved: upgrade of the system needed.

– Photoemission studies on hydrogenation of hydrogen evolution reaction electrodes using the hydrogen membrane approach focus on V, ZrV₂ – achieved.

– Continuation of hydrogenation of gaseous organic compounds with focus on selective conversion ethylene to specific liquid alkanes (jet fuel) – achieved.

2.2.9 Theoretical Chemistry (Prof. S. Luber)

– Continuation of the study of molecular Co-based water reduction catalysts on surfaces: this was not achieved since the project goal was changed.

– Study of the redox potentials for mono- and dinuclear Co-based complexes in collaboration with experimentalists: ongoing project with the Alberto group – calculations are finished, the manuscript still needs to be completed from all participating parties

– Development of an approach for excited state dynamics of condensed phase systems: an efficient approach was developed and published.

2.3 Updated project planning

2.3.1 Photocatalytic Water Reduction: WRCs and Photosensitizers (Prof. R. Alberto)

Water / CO₂ Reduction Catalysts

- Extending dual-core WRCs to cyclic systems based on the pyrphrines and acyclic systems based on mono-anionic bis-pyridyl-nitrile ligands. Combination of advantages of acyclic poly-pyridyl and cyclic pyrphyrin-type ligands.
- Photocatalytic efficiencies of these catalysts for CO₂ and water reduction, electrochemical properties.
- Conjugating anchoring groups to terminal functionalities.

Photosensitizers

- Exchanging the apical halido or hydroxo ligands with electron acceptors and other functional systems.
- Assessing the photo- and electrochemical properties of these Re₆S₈-type clusters as a function of additional apical ligands, solvent, and other physico-chemical parameters.
- Determination of reductive and oxidative quenching with each photosensitizer.
- Introducing anchoring groups to the apical sites for surface grafting.

Further objectives

- Investigations of the full water splitting cell from the collaboration with the company.
- Using this setup for grafting our WRC on the photocathode side of the cell.
- Assessing efficiencies of the model and our own systems for H₂/O₂ formation.

2.3.2 Visible-Light-Driven Water Oxidation Catalysts (WOCs) (Prof. G. R. Patzke)

Design and understanding of chalcogenide-based electrocatalysts for water splitting

In 2021, we identified and mechanistically investigated highly efficient cobalt phosphide-based electrocatalysts for overall water splitting (see also 3.2 on research below). We will now further develop our operando methodology towards a precise understanding of the role of the non-metal centers in the process. The high performance of the initially investigated system is an excellent starting point for investigating optimized materials of the general type A-M-O-M-A (A: P, S, Se, and Te; M: Fe, Co, and Ni). The influence of anionic substitution on the HER performance in alkaline media will be investigated in particular, along with mechanistic and DFT studies.

Exploration of transition metal carbodiimides as catalysts for the oxygen evolution and reduction reactions (OER/ORR)

Based on our published track record in the analysis of cobalt carbodiimide (CoNCN) as photo- and electrocatalysts for water oxidation, we will set out to develop new routes for the growth of MNCN nanoparticles on conductive nanosheet substrates, especially reduced graphene oxide (rGO) or carbon nanotubes (CNTs). Preliminary results (see also research 3.2) show that these composites are also quite promising ORR catalysts. Special emphasis will be placed on their *operando* monitoring with XAS to unravel the underlying mechanisms.

Immobilization and exploration of molecular catalysts for water oxidation and alternative oxidative processes

Starting from our results on the superior role of amorphous cobalt oxide nanoparticles over molecular catalysts in photo-driven OER [26], we will set out to functionalize and immobilize molecular transition metal water oxidation catalysts on electrode surfaces in order to benefit from their manifold design options. As a step beyond water oxidation, we will also start to explore the potential of 3d transition

metal complexes as catalysts for urea oxidation or other alternative processes to water oxidation, both as molecular catalysts or as pre-catalysts for composite materials. This can be connected to planned joint investigations with Ocean University of China (Qingdao) via a visiting CSC PhD scholarship in 2022 (Dan Zhang) concerning the replacement of the OER half reaction with the catalytic decomposition of water pollutants.

Further objectives

GR Patzke plans to strengthen the position of the URPP LightChEC in the Swiss academic and industrial landscape through her memberships in the Swiss Academy of Technical Sciences (SATW), in the Daylight Academy (DLA) and in the scientific advisory board of the AEE Suisse.

2.3.3 Time-resolved Spectroscopy of Artificial Photosynthetic Systems (Prof. P. Hamm)

- In the upcoming year, we will focus on CO₂ reduction, continuing from the current stage of the project that is discussed below. That is, we will consider the second reduction step in the presence of CO₂, in which case CO₂ binds to the catalyst, gets reduced once, and forms a tri-carbonyl complex, according to proposals in the literature. All these intermediates should reveal very characteristic bands in the IR spectrum and should be detectable by transient IR spectroscopy. To that end, we will construct a measurement setup, in which the Ru-catalyst is pre-reduced once in an electrochemical cell. It then will be mixed with all other reaction components in a rapid-mixing device that will also serve as the IR measurement cell.
- Once established for the currently studied catalytic system, we will extend this approach to a wide variety of molecular CO₂ reduction catalysts that might also produce different products (e.g., CO, formate).

2.3.4 Surfaces (Prof. J. Osterwalder)

- Completion of the data analysis for the Ga₂O₃ growth study on Cu₂O(111) and paper writing.
- Growth study of Ga₂O₃ on Cu₂O(110) that should provide a better lattice match to β-Ga₂O₃.
- Continuation of the study of Ni monolayer and sub-monolayer films on Fe₃O₄(001) and the formation of the Ni-ferrite phase via annealing. Structural characterization is already advanced, measurements of the electronic properties are carried out in 2022.
- The two projects will constitute the main content of the PhD thesis of Mert Taskin who will finish his degree at the end of 2022.
- Measurements of the photoexcited charge transfer dynamics in the h-BN/Cu_{2-x}O/Cu(111) system grown by oxygen intercalation into h-BN/Cu(1111).

2.3.5 Molecular Approaches to Renewable Energies (Prof. D. Tilley)

- Sb₂Se₃: alternative synthesis methods for this material will be explored, such as hydrothermal synthesis, and selenization of thermally evaporated thin films of antimony metal. The improvement of the photovoltage will continue to be explored via various methods.
- Impedance spectroscopy: we continue to refine our model and understanding based on the study of different materials. This project will mesh more with the other group projects in the future, helping to understand different Sb₂Se₃ structures, as well as anchored molecular electrocatalysts.
- Immobilization of molecular catalysts via host-guest interactions: we will learn which solvent systems work best for the quartz crystal microbalance (QCMB) and investigate binding and de-binding of guest molecules in anchored hosts on both gold and oxide materials. We will begin our

investigations on electrochemical QCM, to measure mass changes during electrosynthetic reactions.

2.3.6 Computational Studies of Dynamic Properties of Water Oxidation (Prof. J. Hutter)

- We plan to use the generated machine learning potential for the metal-water systems to study water structure and dynamics under potential of zero charge for the different interfaces.
- We will apply path-integral molecular dynamics to address the probability of self-ionization events of water at the interface with metals like Rh, Pd, Ag, Ir, Pt, and Au (possibly also at electrified surfaces).
- The adsorption of metal atoms and metal clusters at the hBN/Cu₂O (111) interface will be considered also as intercalated between the oxide and the overlayer. We will focus on specific reactive processes and on the effects of confinement at the interface.
- We still aim at the simulation of the dynamics of molecules at the interface under the influence of time-dependent fields. The focus is on the application of excited state dynamics, which has been successfully applied in literature to study light-induced processes of aqueous metallic nanoparticles.

2.3.7 Surfaces / H₂ and CO₂ Storage and Conversion (Prof. K.-H. Ernst)

- Study the adsorption/desorption and coordination/activation of CO₂ and CO on MOFs by using FTIR spectroscopy, TDS and possibly ToF-SIMS: We will use isotopically labeled CO₂ and CO to distinguish the adsorbate from the CO-based MOF. Once the adsorption/desorption is understood, hydrogenation using atomic and molecular hydrogen.
- On-surface synthesis of MOFs on graphene/Ru(0001) and creation of 2D MOFs on thin insulating films, such as MgO on Ag(100), in order to understand the properties of the low-D MOFs unperturbed by the metal surface.
- Publication of the synthesis of MOFs on Au(111) along with the magnetism data: Quantitative analysis of the XAS/XLD/XMCD spectra using the real-space crystal-field software "multiX".

2.3.8 Electronic Structure of Materials for Solar-Water Splitting (Dr. A. Borgschulte)

- Continuation of solar water splitting probed by magneto-optics with focus on metal hydride forming electrodes.
- Photoemission studies on hydrogenation of hydrogen evolution reaction electrodes using the hydrogen membrane approach focus on reactive materials such as V, ZrV₂, and classical materials such as Ni and Fe, and Co (-oxides) using hard X-ray photoelectron spectroscopy combined with impedance spectroscopy.
- Continuation of hydrogenation of gaseous organic compounds with focus on selective conversion of ethylene to specific liquid alkanes (jet fuel).

2.3.9 Theoretical and Computational Chemistry (Prof. S. Luber)

- Extension of the excited state dynamics approach to include spin-orbit coupling.
- Study of excited state dynamics of molecules related to artificial photosynthesis.
- Implementation of efficient algorithms in order to improve convergence of the excited state calculations for non-adiabatic dynamics.

3 Research

3.1 Photocatalytic Water Reduction: WRCs and Photosensitizers (Prof. R. Alberto)

The research in 2021 followed four branches; i) preparation and characterization of novel dual core catalysts and investigating their photo/electrocatalytic performance, ii) polymerization of the pentapyridyl catalyst with a thiophene backbone and evaluating photocatalysis with water soluble polymers and electrocatalysis with the polymer grafted on electrodes, iii) the preparation of Mo_3S_x -type catalysts for heterogenization on semiconductors and iv) the preparation and characterization of

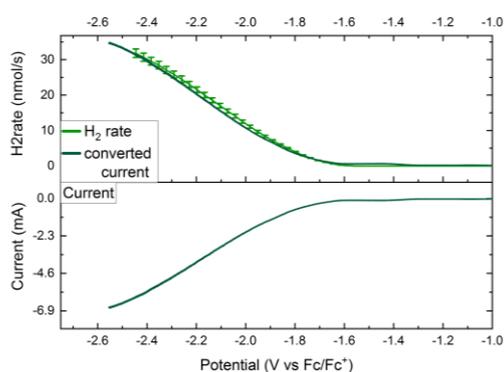


Figure 1: Dual core catalyst, H_2 rate vs. current and Faradaic yield.

the dual cores according to our concept do not bring the expected advantage. We assume this is due to the nature of the catalyst, wherefore we will resume catalysts with tautomeric properties as described above.

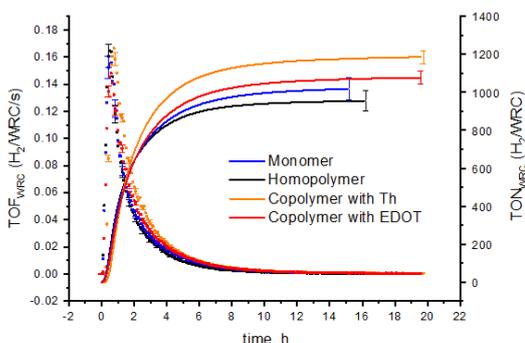


Figure 2: TONs and TOFs of single WRC and (co)polymerized.

Organic conducting polymer backbones conjugated to WRCs represent an entry into organic photocathodes. We prepared different thiophene monomers, carrying the WRC and (co)polymerized them to different molecular weights. Activity of the (water soluble) polymers in solution was the same as of the monomer, confirming that activity is not lost. Grafting the polymers on an ITO cathode gave a long-lived electrocatalysts.

MoS_2 is a well-known catalyst for water reduction. To investigate an atom-precise excerpt of its structure, we prepared clusters of the $[\text{Mo}_3\text{S}_4]^{4+}$ and $[\text{Mo}_3\text{S}_{13}]^{2-}$ core. Both showed some photocatalytic activity. We grafted the clusters on Sb_2Se_3 layers (Tilley) and performed CV to see with XPS (Osterwalder) if the structures remained intact. According to the XPS data, the clusters were oxidized/hydrated rather rapidly and we detected MoO_3 amongst other species on the surfaces of the semiconductor. We conclude that these clusters are not suitable for electrocatalysis and decided not to pursue them.

Clusters of the $[\text{Re}_6\text{S}_8]^{4+}$ type are known since a long time. They have excited state lifetimes in the microsecond range, depending on the additional ligands in the apical positions. They are synthesized at high temperatures (around 1000°C) from the elements in quartz tubes. We succeeded after some drawbacks in the synthesis of $\text{Cs}_5[\text{Re}_6\text{S}_8]\text{Br}_7$. The bromides were exchanged by hydroxide to achieve water-soluble clusters. Whereas the physico-chemical properties of these clusters are well established and look promising for photocatalysis, they have never been investigated for this purpose. Life-time determinations confirmed the long-lived excited states and we found that oxidative quenching in organic solvents is diffusion limited. The next step is to submit these clusters to photocatalytic studies with the goal of having a stable photosensitizer over prolonged times.

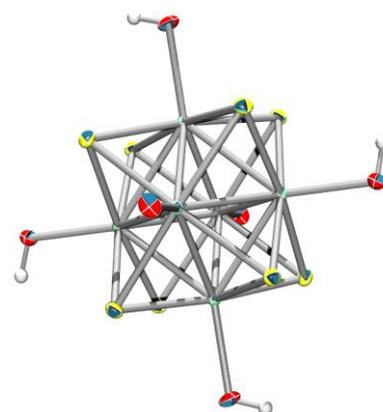


Figure 3: Ellipsoid displacement plot of $[\text{Re}_6\text{S}_8(\text{OH})_6]^{4+}$.

3.2 Visible-Light-Driven Water Oxidation Catalysts (WOCs) (Prof. G. R. Patzke)

Our research on 3d transition metal oxide catalysts was rounded off to a large extent in 2021 through comprehensive publications. Generally, we pursue a dual strategy based on understanding both the formation parameters and pathways of materials as well as their mechanisms of action. Concerning the former, we managed to monitor the structural evolution of permanganate precursor for MnO_x -based OER electrodes with complementary *in situ* heating HR-TEM studies and heating X-ray powder diffraction [14] (Dr. Sima Heidari). The high vacuum conditions of the TEM measurements as well as the thermal energy of the electrons induced a different sequence of oxide phases in the thermal transformation of the KMnO_4 precursor when compared with PXRD measurements. This result underscores the significant influence of the selected monitoring method on the observed reaction pathways - with methodological impact on related studies in the field.

Likewise, our rigorous comparison of the OER performance of benchmark Co-based molecular catalysts and disordered nanoscale *in situ* precipitates of Co-salts revealed that the photocatalytic performance could simply be maximized through self-optimization of such precipitates rather than through their elaborate molecular design [26] (Lukas Reith). Along with the emerging guidelines for tuning Co-oxide OER catalysts through balancing valence, disorder and structural motif, these results are impactful for the ongoing strategic debate about molecular vs. heterogeneous OER catalysts.

Next, our investigations on fluoride etched Ni-based electrodes as economic OER catalysts (Esmael Balaghi) were finally submitted and accepted for publication in 2021. The optimized NiF5% catalyst is competitive with recent Ni-based OER electrocatalysts and further excels in comparison through a minimum of required preparative effort, rendering the material economically attractive. Comprehensive analyses (e.g. XAS, XPS, HR-TEM and electrochemical impedance spectroscopy) attributed the high performance to facilitated electron transfer through the thin porous layer etched onto the Ni surface.

A major research highlight of 2021 was the submission of our study on cobalt phosphide-based electrocatalysts for overall water splitting [22-1] (Yonggui Zhao). We obtained hierarchically structured Co@CoFe-P nanobox (NB) particles through a facile self-templating approach involving yolk-shell ZIF-67@CoFe-Prussian Blue precursors. First, the Co@CoFe-P NBs stand out as high performing electrocatalysts that drive both oxygen and hydrogen evolution over the wide pH range from ca. 0 to 14. Their hierarchical engineering led to particularly low HER overpotentials (e.g. 83 mV at 10 mA cm^{-2} in 0.5 M H_2SO_4) and comparably enhanced OER overpotential values. This resulted in excellent

bifunctionality in overall water splitting settings, where the Co@CoFe-P NBs afforded a current density of 10 mA cm^{-2} at a cell voltage as low as 1.49 V and sustained current densities up to 100 mA cm^{-2} for $> 220 \text{ h}$ with no apparent decline in performance. We proceeded to unravel the restructuring processes and real active species responsible for this industrially attractive performance with a combination of

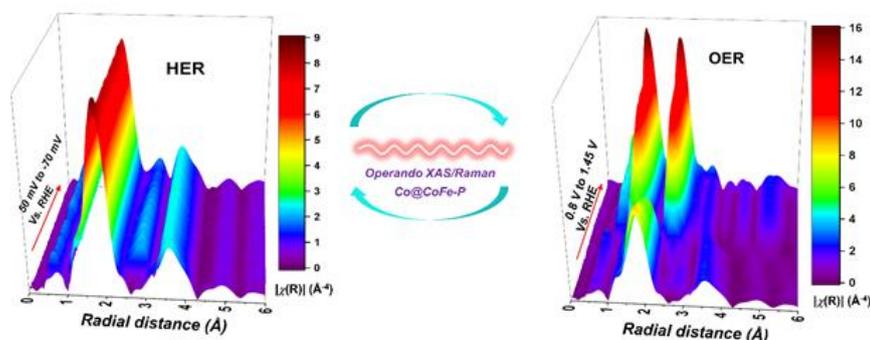


Figure 4: Operando XAS monitoring of HER/OER with hierarchical Co@CoFe-P nanoboxes.

operando XAS and Raman spectroscopy, which was complemented with rotating ring disc electrode (RRDE) experiments. Special emphasis was placed on identifying the active HER species that are usually more elusive than those responsible for OER. Spectroscopic results in their entirety brought forward active P-Co-O-Fe-P configurations with low valent M^0/M^+ metal sites resulting from in situ restructuring of the material. These moieties lowered the energy barriers for water dissociation and H^* adsorption according to our DFT results. The enhanced OER performance of Co@CoFe-P NBs was linked to the facilitated formation of $Co^{III/IV}-O-Fe^{III/IV}$ configurations when compared with Co/Fe-oxyhydroxide references. These substantial insights now pave the way to explore the full spectrum of A-M-O-M-A (A: P, S, Se, and Te; M: Fe, Co, and Ni) systems, which are in principle available through our convenient templating routes.

3.3 Time-resolved Spectroscopy of Artificial Photosynthetic Systems (Prof. P. Hamm)

We have explored in Ref. [25] the photo-induced redox reactions of a rhenium-tricarbonyl complex on a solid-liquid interface, that is embedded in a layer of zirconium oxide deposited by atomic layer deposition (ALD, see Figure 5). Time-resolved and steady state infrared spectroscopy were applied to reveal the correlations between the thickness of the ALD layer and the accessibility of the complex by reductive quencher molecules in solution. We observed a transition of the molecular environment from flexible to rigid, as well as limitations to ligand exchange and excited state quenching on the embedded complexes, when the ALD layer is roughly of the same height as the molecules.

We have furthermore investigated the photo-induced reaction cycle of a molecular CO_2 reduction catalyst. The reaction mixture consisted of the actual catalyst ($trans(Cl)-[Ru(dmbpy)(CO)_2Cl_2]$), as well as a photo-sensitizer ($Ru(dmbpy)(CO)_2Cl_2$), and a sacrificial electron donor (BNAH) in DMF as solvent. So far, we concentrated on the first reduction step, which does not yet enter the CO_2 reduction cycle, but prepares the catalyst by freeing one binding site at the metal center. With the help of time-resolved IR spectroscopy, we could resolve in great detail the kinetics of two Cl ligands leaving and one DMF molecule. A publication is currently being written up.

The photophysics of Re(I) tricarbonyl (Inorg. Chem. **2021**, *60* (3), 1334–1343) and dicarbonyl [10] complexes with substituted terpyridine ligands have been studied in detail with the help of DFT, time-resolved IR and (spectro)electrochemical methods. In the former, introduction of the electron-rich NMe₂ group induces a dramatic increase in absorption and a change in the character of the lowest excited state from MLCT to ILCT, accompanied by an enhancement of the lifetime from 2 ns to 380 ns. This modulation however is absent in the dicarbonyl complexes, which are non-emissive and deactivate within 1 ns, due to the coordination environment being unable to promote ILCT. This work was performed by Ricardo Fernández-Terán and Laurent Sévery in the groups of Prof. Peter Hamm and Prof. David Tilley, respectively, but without any active contribution of the corresponding PIs.

Finally, the solvation of the M–H bond has been studied by 2D-IR spectroscopy, where the spectral diffusion kinetics reveal a long-lived inhomogeneity with a non-monotonic behavior vs. the hydrogen bond acidity/basicity of the solvent, and a monotonic increase as a function of the mole fraction of an acidic alcohol. We believe this effect shows the ambivalent character of the solvation of the hydrides, which adapt their partial charge to the character of the solvent. The manuscript is currently at the writing stage, with some DFT and NMR studies pending to confirm the overall science.

3.4 Surfaces (Prof. J. Osterwalder)

Gallium oxide films are known to improve the performance of cuprous oxide-based photocathodes in PEC cells and are routinely used in the Tilley group. In order to characterize the interface between these two materials, ultrathin films of Ga₂O₃ were prepared in UHV by evaporating Ga metal onto Cu₂O(111) in a low oxygen partial pressure. In order to crystallize the oxide film, post-annealing was performed at increasing temperatures. At a certain threshold temperature, strong interdiffusion starts, resulting in a reduction of the film thickness. Interestingly, the film is more stable when, prior to Ga deposition, the Cu₂O(111) surface is prepared to form the ($\sqrt{3}\times\sqrt{3}$)R30° reconstruction, where every third oxygen atom within the surface layer is missing.

Ni ferrite (NiFe₂O₄) is an interesting earth-abundant catalyst for photocatalytic water oxidation (D. Hong *et al.*, *JACS* **2012**, *134*, 19572). Our group prepares model Ni ferrite catalyst surfaces by first depositing Ni metal to thicknesses ranging from sub-monolayers to several monolayers on top of a Fe₃O₄(001) surface and subsequent annealing. Auger electron diffraction (AED) data measured with the Ni LMM Auger signal reveal the incorporation of the Ni ions into the magnetite lattice (Figure 6). When several monolayers of Ni are deposited, the transition from a metallic Ni film to a Ni ferrite like surface is observed at a temperature of 250°C.

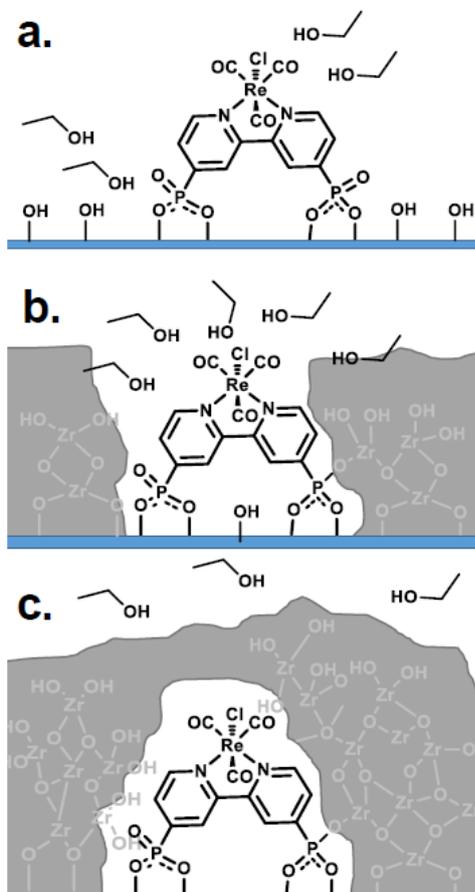
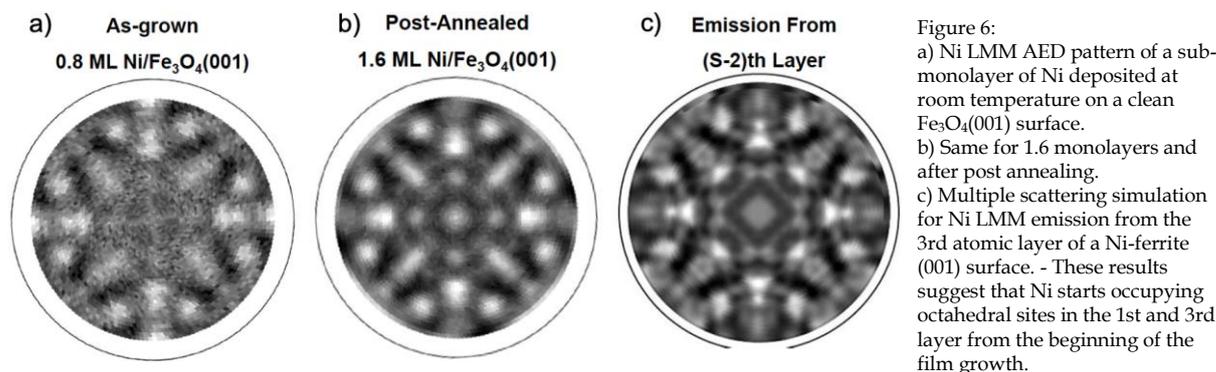


Figure 5: A solid-liquid interface with a rhenium-tricarbonyl complex embedded by an ALD layer of ZrO₂, whose thickness has been varied.



Finally, we succeeded in preparing a cuprous oxide like interlayer underneath a monolayer of h-BN grown on top of Cu(111) via oxygen intercalation. XPS and photoelectron diffraction data confirm that the h-BN layer remains intact, and STM images suggest that the initial oxide sublayer has a similar structure as the one that forms on a bare Cu(111) surface. This system is interesting in view of its promise for confined catalysis in two dimensions, and it is also studied in the Hutter group,

3.5 Molecular Approaches to Renewable Energies (Prof. D. Tilley)

Nearly my entire group is associated with the LightChEC, as all my 3rd party funding is on related topics. In terms of thin film water splitting photocathodes, the two main materials in our lab are antimony selenide (Sb_2Se_3) and copper oxide (Cu_2O). Excellent progress was made on both of these materials. A manuscript on Cu_2O was submitted to a top journal end of 2021, and it is currently in revision. For antimony selenide, two PhD students are working on the topic, with different synthetic approaches. They are both close to their first paper submission. For the impedance topic, a PhD student is trying to more fully understand the impedance spectra that we obtain from multilayer photoelectrodes, and she is making good progress. For the anchored molecular catalyst work, a further paper was submitted end of 2021, and finally published in Jan 2022. [22-2]

3.6 Computational Studies of Dynamic Properties of Water Oxidation (Prof. J. Hutter)

The work in our group aims at the atomistic understanding of structure/property relations as well as of processes and catalytic mechanisms involving functional materials of interest in photocatalysis and electrochemistry. To this purpose we employ electronic structure calculations also combined with ab initio molecular dynamics. Some of the projects are inspired by the collaboration with other groups in the consortium, e.g., Osterwalder's group. On the other hand, we also propose model systems that allow a more in-depth investigation of some fundamental aspects, as specific properties of interfaces, spectroscopic features of adsorbates, dynamics at surfaces.

We generate empirical potentials to simulate water/metal by applying machine learning procedures based on density functional theory datasets. The proposed workflow goes over the following steps

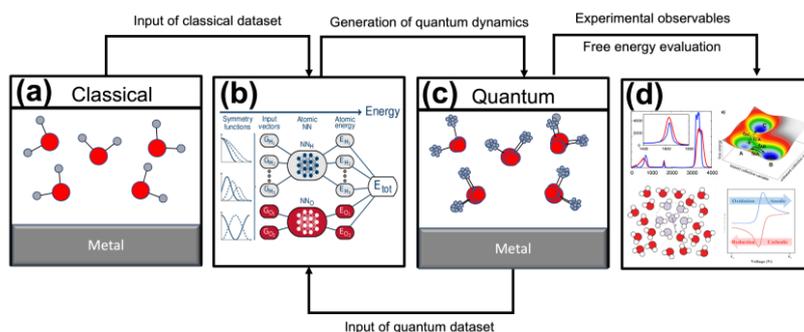


Figure 7: Proposed workflow to understand the alkali metal cations effects at electrochemical interfaces using (path-integral) AIMD accelerated by a machine learning approach. (a) Generation of initial datasets using classical molecular dynamics. (b) Development of potential based on machine learning. (c) Inclusion of nuclear quantum effects. (d) Calculations of free energy landscapes and experimental observables.

shown in Figure 7: a) Generate ab-initio molecular dynamics trajectories of about ten picoseconds; b) Train a machine learning potential based on those datasets; c) Extend the phase space using path-integral molecular dynamics based on machine learning potential and apply active learning procedures to refine the potential. d) Predict the properties at electrochemical interface and

calculate experimental observables. This generalized automated machine learning potential generator will be released, to be extended and applied to a variety of electrochemical problems.

We studied in more details the electronic properties of the Cu_2O (111) surface owing to the presence of oxygen vacancies placed at different sites in the top or sub surface layers. For this investigation we compared different DFT-approximations, including the Hubbard model (DFT+U varying U) and hybrid functionals. We assessed the DFT approaches on bulk and surface models of the cuprous oxide. The (111) surface is known to be stabilized by the removal of the topmost unsaturated copper atoms. The resulting deficiency of copper induces the presence of localized acceptor levels and the presence of polarons at the surface and subsurface layers. DFT+HSE06 reproduces well the experimental findings. The oxygen vacancy formation energies at different sites are found to depend strongly on the applied functionals. The different functionals yielded conflicting results. However, they agreed that the oxygen vacancy located at the surface is less stable than the oxygen vacancy located within the subsurface layer. Using HSE06 we could also demonstrate that the formation of an oxygen vacancy is accompanied by the presence of polarons, which can as well be located at the surface or in the subsurface layer. This suggests an increased mobility of electrons on the surface regardless of their position.

The hydrophilic UV-induced effect of the titanium dioxide surface can be related to the oxidation of adsorbates. Moreover, the formation of mixed formate/acetate monolayers transforms the initially hydrophilic surface into a hydrophobic one. These monolayers give rise to a (2x1) surface reconstruction on TiO_2 (110). However, experimental studies indicate that, once the TiO_2 (110) + formate surface is exposed to water, the initial (2x1) surface superstructure is lost. The timescale of the process depends on the water pressure to which the system is exposed. Following our static DFT studies to characterize the structural and electronic properties of the monolayer under dry as well as humid conditions, we employed DFT molecular dynamics to take into account temperature and dynamic effects.

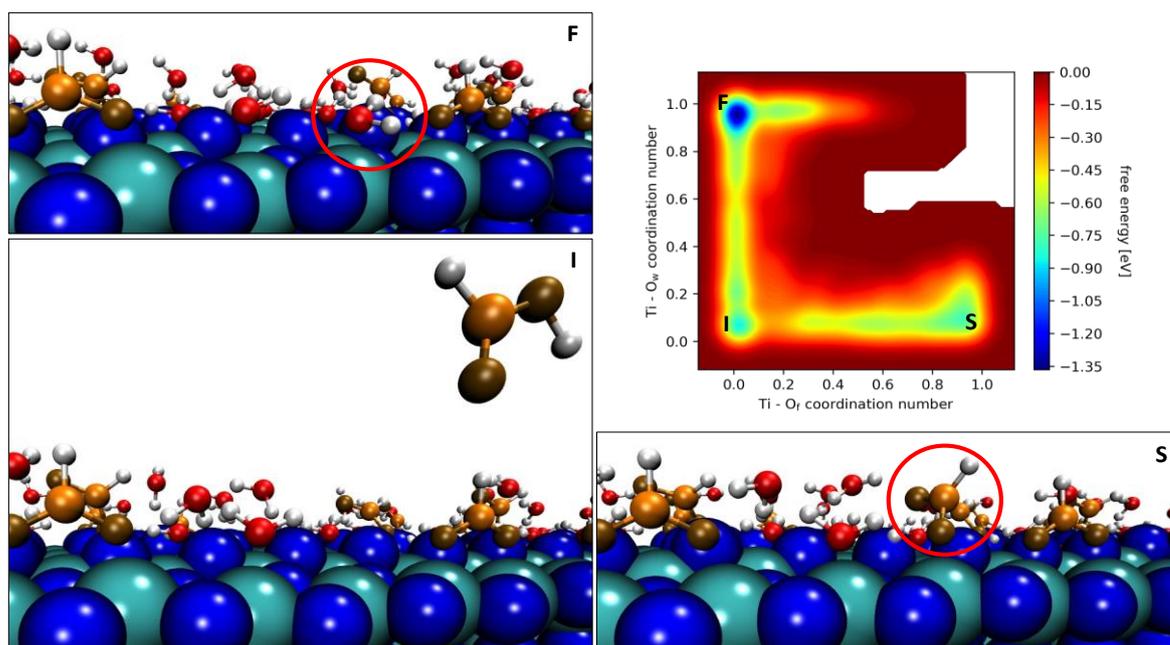


Figure 8: Water-to-formate replacement process. The ball and stick representations correspond to snapshots extracted from the trajectory, at three different regions of the free energy landscape, labelled S, I, and F. The corresponding free energy map is shown as a function of two order parameters, which describe the coordination of the surface with water and with formate.

Metadynamics simulations (Figure 8) have been also performed to enhance the sampling and address the probability of transformation processes. Starting from different initial configurations of the co-adsorbed formate and water on rutile (110), we have been able to show that the added water molecules perturb the formate superstructure by replacing some of the adsorbed formate radicals. The process happens in two steps, as the reconstructed free energy surface shows: i. first the formate radical binds to a hydrogen atom (from a water molecule or bridging OH) and desorbs, leaving an unsaturated Ti site behind; ii. a water molecule approaches this Ti site, binding to the surface. The processes have free energy barriers of 0.42 and 0.18 eV, respectively, which indicates that the substitution takes a relative short time to occur, but it is not instantaneous.

3.7 Surfaces / H₂ and CO₂ Storage and Conversion (Prof. K.-H. Ernst)

Low-dimensional metal-organic frameworks (MOFs) constitute a very versatile class of nanomaterials whose electronic, magnetic, and catalytic properties can be tuned by choice of the metal atom and the ligand. Oxocarbons, a class of ligands consisting only of oxygen and carbon, represent ideal molecules to produce metal-rich MOFs which have a high density of catalytically active sites.

Here we report on the on-surface synthesis of Co, Ni and Er-based MOFs using the ligand squarate (C₄O₄²⁻) on Au(111). The materials are studied by STM (Scanning Tunneling Microscopy), XPS (X-ray Photon Spectroscopy) and XAS/XLD/XMCD (X-ray Absorption Spectroscopy, X-ray Linear Dichroism, X-ray Magnetic Circular Dichroism) and TDS (Thermal Desorption Spectroscopy).

XPS is used to analyze the formation of Co-, Ni-, and Er-squarate layers. Figure 9 shows C 1s and O 1s XP spectra of SqA multilayer on Au(111) and the corresponding MOFs. Upon M addition (M = Co, Er) and annealing (100°C), the multilayer is desorbed leaving behind a single layer of molecules. In the case of O 1s, the presence of only one peak (at 531.4 eV) corresponding to C=O, proves the two-fold dehydrogenation of SqA and the formation of squarate (Sq).

XPS data of the {Ni,Co,Eu,Er}Sq MOFs show that Co and Ni are in +II oxidation states. Interestingly, Ni 2p XP peaks strongly suggest that Ni is in a high-spin ($S = 1$) state. Eu and Er are identified as formal +III ions.

The STM images of the MOFs reveal dense layers for NiSq and CoSq. The layers consist of condensed arrays of TMSq wires (Figure 10a). In case of ErSq, STM reveals a sparse arrangement (Figure 10b). Further STM investigations and STM modeling of RESq MOFs are work in progress. We expect that the sparse arrangement is the consequence of the formal oxidization state of the RE (+III) and ligand (-II) which implies a RE_2SQ_3 stoichiometry or the presence of a radical as in case of RE double-decker phthalocyanines. STM shows very short M-M distances of 5.5 Å and 5.6 Å in TM and RE squarate MOFs, respectively.

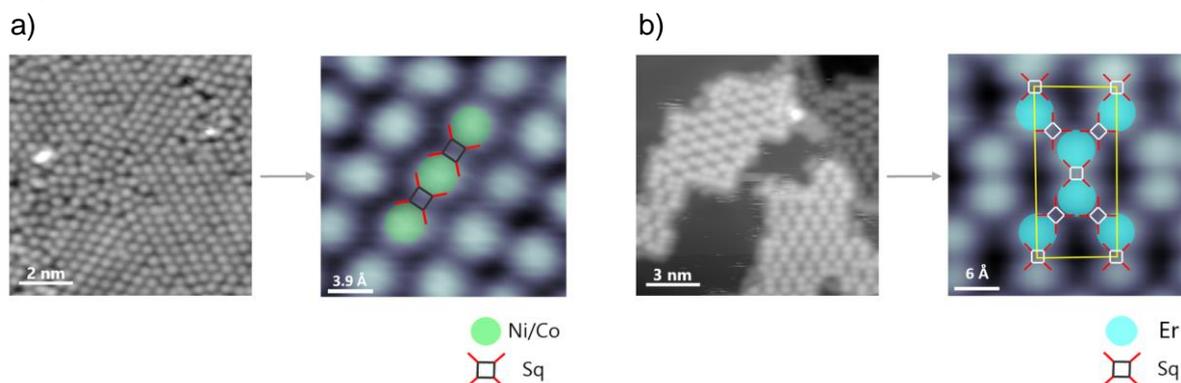


Figure 10: a) STM data. SqNi forming condensed arrays of molecular wires, and the proposed structural model. b) SqEr forming sparse structures, and the proposed structural model.

The magnetic properties of MOFs bearing transition metals and rare earth elements were measured at the XTreme beamline of the Swiss Light Source of the Paul Scherrer Institute. TM L edge and RE M edge XAS and XMCD obtained at 6.8 and 3 K in grazing and normal incidence reveal the magnetism of the MOFs.

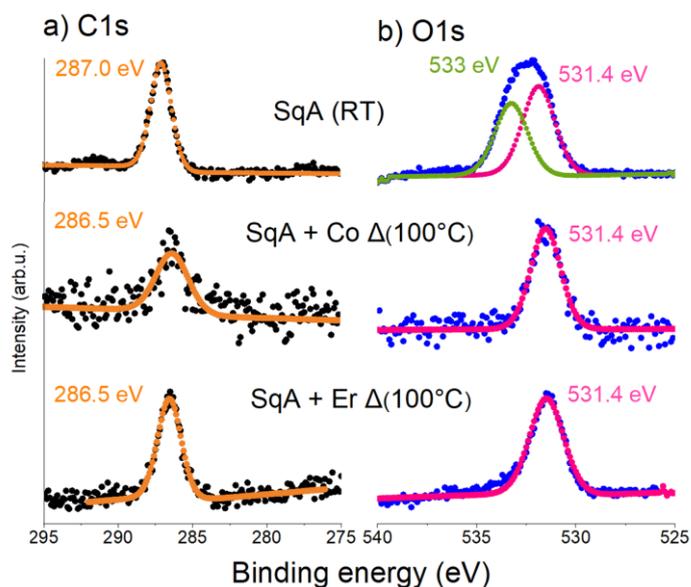


Figure 9: XPS spectra showing transition from SqA multilayer to 2D squarate MOFs on Au(111). C 1s (a) and O 1s (b) peaks show a shift to lower binding energies upon Co- and Er-squarate complex formation.

Ni L edge XAS/XMCD shows the presence of paramagnetic Ni (i.e. high spin) in NiSq with a weak out-of-plane easy axis of magnetization (Figure 11a). Co L edge XAS/XMCD evidences a significant in-plane magnetic easy-plane/easy axis (Figure 11b). Er shows a high magnetization but a very low magnetic anisotropy (data not shown). In particular the formation of high-spin Ni complexes is rather surprising and points towards a significantly non-planar coordinating sphere.

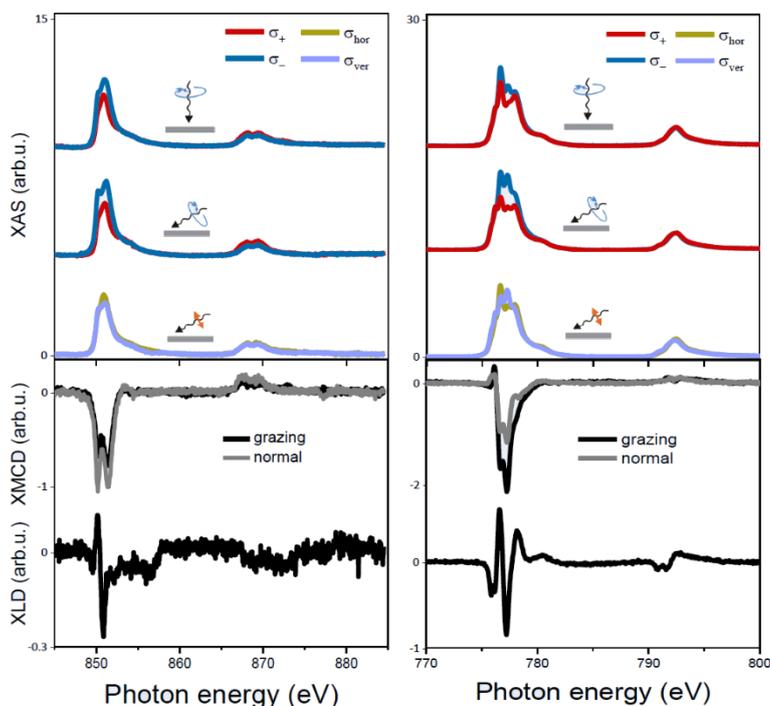


Figure 11: X-ray spectra of a monolayer of a) NiSq and b) CoSq on Au(111), revealing the magnetic anisotropy and the orientation of the molecules.

X-ray absorption spectra (XAS) are acquired at 3 K using circularly and linearly polarized X-rays were obtained in normal and grazing incidence in an applied field of 6.8 T. Their difference, XMCD, is a direct measure of the magnetic moment of Ni and Co. The X-ray linear dichroism (XLD), the difference of the linear polarized XAS, is obtained at 0.1 T in grazing incidence.

In addition, the O K edge XLD is very well suited to determine the chemical state and orientation of the squarate ligands. We find that all MOFs studied (Co, Ni and Er) the ligands are strictly oriented parallel to the surface.

TPR shows that the MOFs decompose into CO, leaving behind a clean surface (XPS data not shown). The up-shift and narrowing of the TPR spectra evidences an autocatalytic decomposition mechanism.

3.8 Electronic Structure of Materials for Solar-Water Splitting (Dr. A. Borgschulte)

In the previous year, we demonstrated the use of magneto-optics for probing HER electrodes designed specifically to match the capabilities of the newly developed setup (Co-Pt superlattices). However, the strongest effect is expected for metal hydride forming electrodes such as TbCo and TbFe. Unfortunately, the field strength of the developed electromagnet turned out to not be strong enough to switch the magnetisation in the films as mandatory for meaningful magneto-optical spectroscopy. Currently, the instrument is upgraded to higher fields to enable the study of more materials.

After an approximately three year instrument development phase financed by the SNF, the research on surface properties of metal hydrides is generating fascinating new results. In a first paper, we

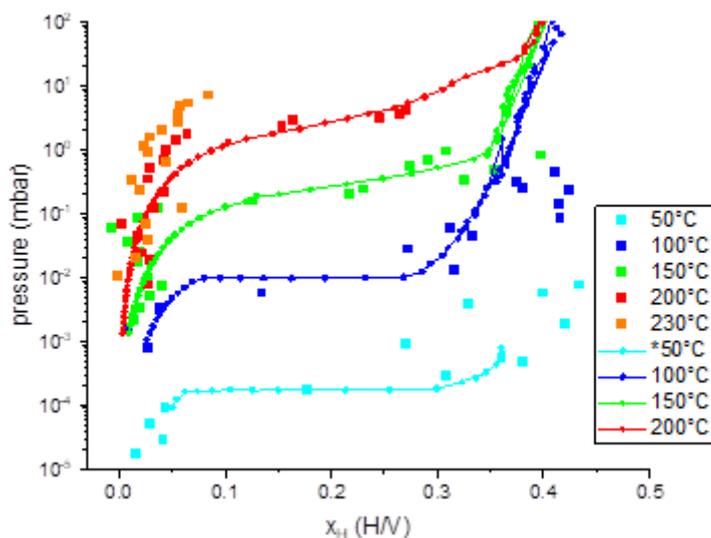


Figure 12: Surface pressure composition isotherms of VH_x measured by the membrane electron spectroscopy setup (squares) compared to literature data (Fukai, Y. *The Metal-Hydrogen System*; Springer-Verlag: Berlin, Heidelberg, 1993).

demonstrated the general feasibility of measuring surface composition isotherms of metal hydrides by electron spectroscopy on the important example TiH_x . From a technical perspective, vanadium is an interesting membrane material, and the experimental setup resembles the membrane application. Figure 12 shows the obtained surface pressure-composition isotherms matching bulk reference data. The good agreement is evidence for the validity of the assumption that the chemical potential at the surface is controlled by the applied pressure on the feed side.

This assumption is basic prerequisite of the analysis procedure. However, it also represents a significant reduction of the permeation through composite membranes as a potential application. Further spectroscopic details indicate a surface depletion layer in VH_x , which is an additional barrier for permeation.

Production of renewable jet fuel from CO_2 and water is an important process on the route to CO_2 -neutral long-distance travel. Our part of the joint PSI-Empa project is the conversion to long chain hydrocarbons of ethylene, carbon monoxide and hydrogen as intermediates formed within the first electrochemical production step. The first year of the project was dedicated to the assembly of the catalytic reactor and analysis techniques for various organic compounds generated during reaction. The production analysis is challenging due to the simultaneously generated gaseous as well as liquid products, and it is tackled by a combination of on-line gas chromatography and NMR.

3.9 Theoretical and Computational Chemistry (Prof. S. Luber)

As one direction, we have studied in detail the RuO_2 water oxidation catalyst. We performed a proper modelling of the RuO_2 bulk and RuO_2 -(110) solid compounds including the presence of an explicit liquid water environment and its dynamics. An accurate description of the bulk RuO_2 properties, such as the lattice parameters of the RuO_2 unit cell and bulk modulus have been monitored resulting in a very good agreement with experimental data. The wettability and the H-bond interfacial environment for the (110)- RuO_2 surface have been studied in the surface reconstruction and accordingly in the chemical activity of the surface [8][9].

Moreover, coupling spin-polarized DFT-MD with state-of-the-art well-tempered (WT) metadynamics we quantitatively assessed free-energy barriers behind the OER at the (110)- RuO_2 catalyst surface revealing plausible pathways composing the reaction network of the O_2 evolution and identify possible catalyst sites without ambiguity. Interestingly, comparing gas-phase and liquid-phase OER free-energy surfaces (FESs), an unprecedented OER pathway with low free energy barrier has been found in the

liquid phase. Remarkably, we found that water molecules thus do not act as a 'guest' but they are explicitly involved in the lowest free-energy OER mechanism identified: in particular, one dissociated water hydrogen hops toward a neighbor water molecule of the surrounding water environment (see Figure 13). This suggests that the synergistic effect between surface catalyst and explicit water environment dynamics is an important and not-negligible basis for a rational design of novel catalysts based on non-precious materials in the context of sunlight-driven artificial photosynthesis.

As another direction, we have developed further our previously presented efficient excited state dynamics approach in order to study non-adiabatic dynamics, also for the condensed phase (mainly liquids up to now). This has for the first time been combined with subsystem DFT, showing that this combined approach provides further computational speed up while still retaining reasonably good accuracy for the excited state dynamics and calculated photoproducts and lifetimes.

Last but not least, we have described a methodology to calculate Raman spectra for liquids both for off- and on-resonance cases in a dynamic setup, paving the way for novel description beyond the standard off-resonance Raman calculations for condensed phase systems or the commonly used more approximate static approach (*J. Chem. Theory Comput.* **2020**, *17*, 1, 344–356).

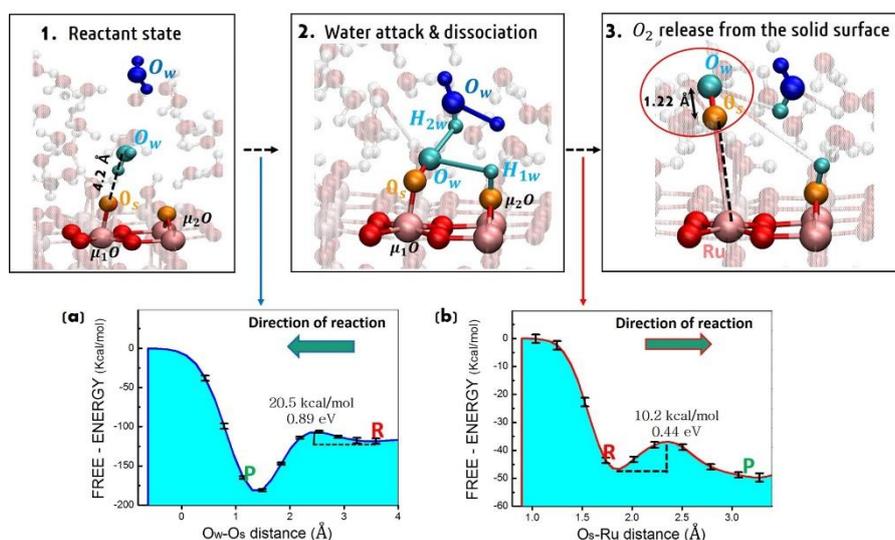


Figure 13: Water-assisted OER pathway at the (110) RuO₂-liquid water interface by means of DFT-MD metadynamics computer simulations.

4 Scientific Activities and Outreach

4.1 Scientific Activities

The URPP LightChEC serves as an exchange platform for all researchers working on the topic of water splitting at the University of Zurich, Empa and PSI. Researchers in positions not funded by the URPP also regularly take part in scientific activities of LightChEC. Around 60 people are part of this scientific community, ten of which were directly employed by the URPP in mid-2021.

Scientific Seminars

As in previous years, the URPP's science seminars were integrated into the Department of Chemistry seminars and highlighted as "LightChEC Co-Seminars".

Four speakers were invited on behalf of LightChEC in 2021:

While the talks in spring were held virtually via Zoom, after the summer break, with the introduction of the Covid certificate at UZH, we could once again invite the speakers to the university campus.

– 27 April: Dr. Emiliana Fabbri, Paul Scherrer Institute, CH

"Insight into Perovskite Oxide Electro-Catalysts as Oxygen Electrodes for Alkaline Electrolyzers"

– 11 May: Prof. Dr. Charles McCrory, University of Michigan, USA

"The Electrochemical Conversion of CO₂ to CO with Polymer-Encapsulated Co Catalysts: Modulating Activity and Selectivity by Controlling the Catalyst's Coordination Environment"

– 21 September: Dr. Roland Hany, Empa, CH

"Carrier Tunneling from Charge Transfer States in Organic Photovoltaic Cells"

– 9 November: Prof. Dr. Julia Kunze-Liebhäuser, Leopold-Franzens University Innsbruck, AT

"Copper Single Crystal Electrocatalysts: Interfacial Structure and Reactivity"

Discussion Meetings

The long-standing series of internal LightChEC Discussion Meetings continued on a monthly basis. These meetings are meant to stimulate exchange and discussions within the LightChEC consortium. Members and associates are encouraged to present interesting research articles, methods, or new concepts to the community, followed by a discussion about the topic.

Although voluntary, the meeting is usually well attended by 20 to 30 people, including many of the PIs. In addition to giving researchers an opportunity to practice scientific presentation skills, the discussion meeting also introduces new concepts, establishes a culture of discussion and thus strengthens the joint spirit of the consortium across the different groups.

During the spring semester, the meetings took place in a video call format, until they were converted back to on-site meetings in autumn, after University of Zurich had implemented the "3G rule" with Covid certificates.

LightChEC Symposium

On 19 November, the LightChEC Symposium 2021 took place. For this symposium, six external speakers were invited to give a talk on one aspect of the broad field of artificial or semi-artificial photosynthesis.

The program also included a poster session, where 24 posters were presented and discussed. Most of them were created by LightChEC researchers, and two external PhD students even presented their work from Germany.

While the list of attendants (68 people) was slightly shorter compared to previous editions, the event can be regarded a major success. Several participants and speakers were happy to take part in person as especially informal discussions and poster presentations are still perceived as more fruitful in face-to-face conversations than through video conferences. Nevertheless, we also seamlessly integrated two

speakers from abroad virtually, making the LightChEC Symposium 2021 a hybrid event. This format can probably serve as a model for future events also for our URPP, where we do not want to do completely without in-person interaction, while avoiding long-distance travel for short events.

Invited speakers and their talks:

- Dr. Carolina Gimbert Suriñach, Universitat Autònoma de Barcelona, ES
"Molecular Systems for Water Splitting"
- Prof. Dr. Evert Jan Meijer, Faculty of Science, University of Amsterdam, NL
"Understanding Solvent Effects in Catalysis"
- Prof. Avner Rothschild, Department of Materials Science and Engineering, Technion, IL
"Wasted Photons: Photogeneration Yield and Charge Carrier Collection Efficiency of Metal Oxide Photoanodes for Photoelectrochemical Water Splitting"
- Prof. Dr. Martin Sterrer, Institute of Physics, University of Graz, AT
"Charge Transfer at Metal/Oxide/Organic Interfaces"
- Dr. Timmy Ramirez-Cuesta, Neutron Sciences, Oak Ridge National Laboratory, USA
"Inelastic Neutron Scattering in Chemistry and Catalysis"
- Dr. Jenny Zhang, Department of Chemistry, University of Cambridge, UK
"Photosynthesis on an Electrode"

4.2 Outreach Activities

The **LightChEC website** recorded about 4'800 visits in the reporting year, which is 28% more than in the previous year. Just over half the visitors registered are from Switzerland, followed by 10% from the USA. The average visit duration has also increased by 26% compared to 2020.

More and longer visits can likely be attributed to the fact that, with the LightChEC Seminar, an event took place again in the reporting year. The *Symposium Program* page was clearly the one most visited, with just under 600 unique page views, most of them in October and November 2021. Other popular pages were *About us*, *Research*, and *Researchers*.

The LightChEC **Twitter** account, set-up in summer 2020, was regularly used during the reporting year to post about new publications, successful defences from our PhD students, and events. As we address a rather specific scientific topic, the audience mostly consists of other researchers. The account has a small number of just over 100 followers thus far, but the level of engagement is considerable at about 2–4 percent per tweet.

The goal for the next year is to reach a broader audience, still writing about new publications in an easily understandable language and additionally posting more general news linked to water splitting and artificial photosynthesis.

Greta R. Patzke contributed a chapter on Artificial Photosynthesis to the 2021 **SATW Technology Outlook**, which was actively promoted on social media. She then continued to present the topic in the "Science after Noon" (online) event of the SCNAT on 12 November 2021.

The **Osterwalder group** has prepared a video clip (<https://tube.switch.ch/videos/b98cf1bd>) presenting their research. It is being displayed on the website of the Department of Physics: physik.uzh.ch/en/research/videos/Condensed-Matter-Physics.html

Sandra Luber appeared in an article in the Swiss magazine **Beobachter** (22.10.2021): "Augenzeugin: «Ich will nachbauen, was Pflanzen tun»".

She also has been interviewed by the **Swiss National Supercomputing Center** CSCS as a guest in the series "Zoom on Science" (online) on 29 October: cscs.ch/publications/stories/2021/zoom-on-science-sandra-luber-chemistry.

5 Academic Career Development

5.1 Activities in Academic Career and Development

Related to the research in the Patzke group, **Lukas Reith** defended his PhD thesis and proceeded to a postdoctoral position at TU Berlin. After his PhD defence, **Esmael Balaghi** moved on to a postdoctoral position at the University of Freiburg (Germany), together with Dr. **Sima Heidari**.

Lisa Grad (Osterwalder group) has successfully defended her PhD degree and has taken a position at Inficon in Balzers (Li).

In the Hamm group, **Ricardo Fernández-Terán** and **Gökcen Tek** both defended their PhD project in 2021 and moved on for postdoc positions at the University of Sheffield and the AMOLF Institute (Amsterdam), respectively.

Dr. **Thomas Moehl** was promoted to a permanent position (Wissenschaftlicher Mitarbeiter) in the group of Prof. David Tilley. Ms. **Jihye Suh** received her PhD in the Tilley group. Dr. **Wooseok Yang** left the Tilley group to start his independent career as a Professor in Sungkyunkwan University (SKKU), a highly ranked University in South Korea.

5.2 Gender Equality Development

In 2021, Prof. Patzke continued to serve as MNF representative of the UZH Gender Equality Commission and as a member of the MNF Gender Equality Committee.

A female PhD student, working on LightChEC projects, was hired in the Tilley group, one in the Ernst group, and one in the Borgschulte group.

In the whole consortium, of the 67 researchers who were part of LightChEC during (most of) the year 2021, 43 were male, 25 were female. This ratio is very similar to the year before, when there were 45 male and 24 female members.

We are happy that artificial photosynthesis generally seems to be a scientific topic that is highly attractive to women researchers.

6 Publications

6.1 List of Publications

23 open access publications 

- [1] Abdi, Z.; **Balaghi, S. E.**; Sologubenko, A. S.; Willinger, M.-G.; Vandichel, M.; Shen, J.-R.; Allakhverdiev, S. I.; **Patzke, G. R.**; Najafpour, M. M. Understanding the Dynamics of Molecular Water Oxidation Catalysts with Liquid-Phase Transmission Electron Microscopy: The Case of Vitamin B12. *ACS Sustainable Chem. Eng.* **2021**, *9* (28), 9494–9505. <https://doi.org/10.1021/acssuschemeng.1c03539>.
- [2] **Balaghi, S. E.**; Mehrabani, S.; Mousazade, Y.; Bagheri, R.; Sologubenko, A. S.; Song, Z.; **Patzke, G. R.**; Najafpour, M. M. Mechanistic Understanding of Water Oxidation in the Presence of a Copper Complex by In Situ Electrochemical Liquid Transmission Electron Microscopy. *ACS Appl. Mater. Interfaces* **2021**, *13* (17), 19927–19937. <https://doi.org/10.1021/acsami.1c00243>.
- [3] **Billeter, E.**; **Sterzi, A.**; Aribia, A.; Grazioli, C.; Coreno, M.; **Bleiner, D.**; **Borgschulte, A.** Hydrogen Induced Trap States in TiO₂ Probed by Resonant X-Ray Photoemission. In *International Conference on X-Ray Lasers 2020*; SPIE, **2021**; Vol. 11886, pp 236–244. <https://doi.org/10.1117/12.2591982>. 
- [4] **Billeter, E.**; Łodziana, Z.; **Borgschulte, A.** Surface Properties of the Hydrogen–Titanium System. *J. Phys. Chem. C* **2021**. <https://doi.org/10.1021/acs.jpcc.1c08635>. 
- [5] **Billeter, E.**; **Sterzi, A.**; **Sambalova, O.**; **Wick-Joliat, R.**; Grazioli, C.; Coreno, M.; Cheng, Y.; Ramirez-Cuesta, A. J.; **Borgschulte, A.** Hydrogen in Tungsten Trioxide by Membrane Photoemission and Density Functional Theory Modeling. *Phys. Rev. B* **2021**, *103* (20), 205304. <https://doi.org/10.1103/PhysRevB.103.205304>.
- [6] **Borgschulte, A.**; **Sambalova, O.**; **Billeter, E.**; **Sterzi, A.**; Niggli, J.; Welte, B.; Heel, A.; Holzner, R. Cataluminescence in Er-Substituted Perovskites. *Adv. Sci.* **2021**, *8* (19), 2101764. <https://doi.org/10.1002/advs.202101764>. 
- [7] **Chen, H.**; **Li, J.**; **Yang, W.**; **Balaghi, S. E.**; **Triana, C. A.**; **Mavrokefalos, C. K.**; **Patzke, G. R.** The Role of Surface States on Reduced TiO₂@BiVO₄ Photoanodes: Enhanced Water Oxidation Performance through Improved Charge Transfer. *ACS Catal.* **2021**, 7637–7646. <https://doi.org/10.1021/acscatal.1c00686>.
- [8] **Creazzo, F.**; **Luber, S.** Explicit Solvent Effects on (110) Ruthenium Oxide Surface Wettability: Structural, Electronic and Mechanical Properties of Rutile RuO₂ by Means of Spin-Polarized DFT-MD. *Appl. Surf. Sci.* **2021**, *570*, 150993. <https://doi.org/10.1016/j.apsusc.2021.150993>. 
- [9] **Creazzo, F.**; **Luber, S.** Water-Assisted Chemical Route Towards the Oxygen Evolution Reaction at the Hydrated (110) Ruthenium Oxide Surface: Heterogeneous Catalysis via DFT-MD & Metadynamics Simulations. *Chem. Eur. J.* **2021**, *n/a* (n/a). <https://doi.org/10.1002/chem.202102356>. 
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- [11] Gouda, L.; **Sévery, L.**; **Moehl, T.**; Mas-Marzá, E.; **Adams, P.**; Fabregat-Santiago, F.; **Tilley, S. D.** Tuning the Selectivity of Biomass Oxidation over Oxygen Evolution on NiO–OH Electrodes. *Green Chemistry* **2021**, *23* (20), 8061–8068. <https://doi.org/10.1039/D1GC02031E>. 

- [12] **Grad, L.**; von Rohr, F. O.; Hengsberger, M.; **Osterwalder, J.** Charge Carrier Dynamics and Self-Trapping on Sb₂S₃(100). *Phys. Rev. Materials* **2021**, 5 (7), 075401. <https://doi.org/10.1103/PhysRevMaterials.5.075401>. 
- [13] Güttinger, R.; Wiprächtiger, G.; Blacque, O.; **Patzke, G. R.** Co/Ni-Polyoxotungstate Photocatalysts as Precursor Materials for Electrocatalytic Water Oxidation. *RSC Adv.* **2021**, 11 (19), 11425–11436. <https://doi.org/10.1039/D0RA10792A>. 
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- [17] **Li, J.**; **Triana, C. A.**; **Wan, W.**; **Saseendran, D. P. A.**; **Zhao, Y.**; **Balaghi, S. E.**; **Heidari, S.**; **Patzke, G. R.** Molecular and Heterogeneous Water Oxidation Catalysts: Recent Progress and Joint Perspectives. *Chem. Soc. Rev.* **2021**. <https://doi.org/10.1039/D0CS00978D>. 
- [18] **Li, J.**; **Chen, H.**; **Triana, C. A.**; **Patzke, G. R.** Hematite Photoanodes for Water Oxidation: Electronic Transitions, Carrier Dynamics, and Surface Energetics. *Angew. Chem. Int. Ed.* **2021**. <https://doi.org/10.1002/anie.202101783>.
- [19] **Li, J.**; **Wan, W.**; **Triana, C. A.**; **Chen, H.**; **Zhao, Y.**; **Mavrokefalos, C. K.**; **Patzke, G. R.** Reaction Kinetics and Interplay of Two Different Surface States on Hematite Photoanodes for Water Oxidation. *Nat. Commun.* **2021**, 12 (1), 255. <https://doi.org/10.1038/s41467-020-20510-8>. 
- [20] **Mattiat, J.**; **Luber, S.** Recent Progress in the Simulation of Chiral Systems with Real Time Propagation Methods. *Helv. Chim. Acta* **2021**, 104 (12), e2100154. <https://doi.org/10.1002/hlca.202100154>. 
- [21] Naik, J. M.; Ritter, C.; Bulfin, B.; Steinfeld, A.; Erni, R.; **Patzke, G. R.** Reversible Phase Transformations in Novel Ce-Substituted Perovskite Oxide Composites for Solar Thermochemical Redox Splitting of CO₂. *Adv. Energy Mater.* **2021**, 11 (16), 2003532. <https://doi.org/10.1002/aenm.202003532>. 
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- [23] **Nikolic, M.**; Daemen, L.; Ramirez-Cuesta, A. J.; Xicohtencatl, R. B.; Cheng, Y.; Putnam, S. T.; Stadie, N. P.; Liu, X.; **Terreni, J.**; **Borgschulte, A.** Neutron Insights into Sorption Enhanced Methanol Catalysis. *Top Catal.* **2021**. <https://doi.org/10.1007/s11244-021-01461-w>. 
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- [38] **Yang, W.; Zhang, X.; Tilley, S. D.** Emerging Binary Chalcogenide Light Absorbers: Material Specific Promises and Challenges. *Chem. Mater.* **2021**, *33* (10), 3467–3489. <https://doi.org/10.1021/acs.chemmater.1c00741>.
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The following publications are referenced in this 2021 report but published only in 2022:

- [22-1] **Zhao, Y.**; Dongfang, N.; **Triana, C. A.**; Huang, C.; Erni, R.; **Wan, W.**; **Li, J.**; Stoian, D.; Pan, L.; Zhang, P.; **Lan, J.**; **Iannuzzi, M.**; **Patzke, G. R.** Dynamics and Control of Active Sites in Hierarchically Nanostructured Cobalt Phosphide/Chalcogenide-Based Electrocatalysts for Water Splitting. *Energy Environ. Sci.* **2022**. <https://doi.org/10.1039/D1EE02249K>. 
- [22-2] Bühler, J.; Zurflüh, J.; Siol, S.; Blacque, O.; **Sévery, L.**; **Tilley, S. D.** Electrochemical Ruthenium-Catalysed C–H Activation in Water through Heterogenization of a Molecular Catalyst. *Catal. Sci. Technol.* **2022**. <https://doi.org/10.1039/D1CY01999F>. 

7 Structures

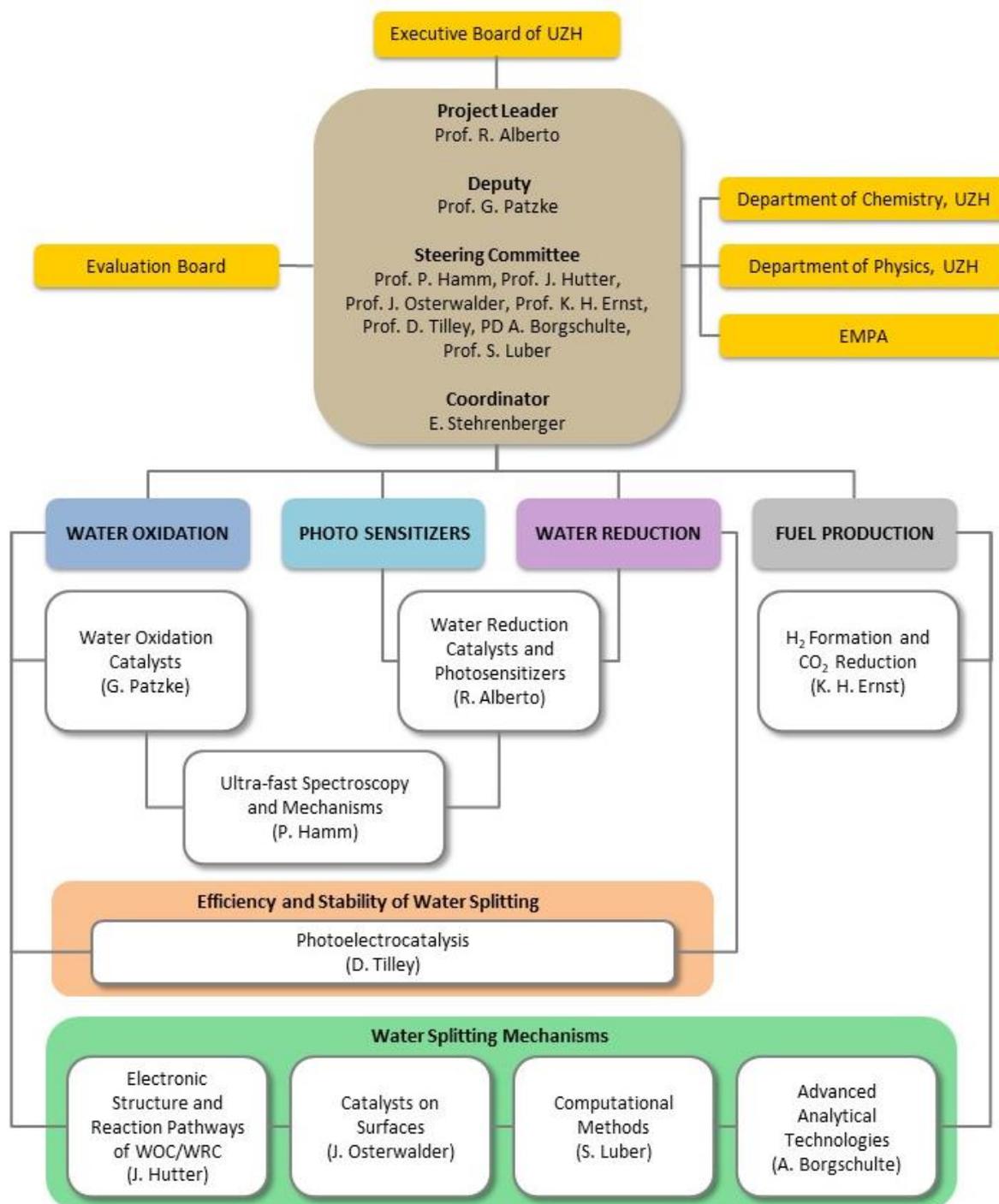


Figure 14: Organizational structure of the URPP LightChEC in 2021.

The URPP structure has remained mainly the same as before. Eva Stehrenberger is the coordinator since December 2020. Starting in 2021, Prof. Patzke will replace Prof. Alberto as project leader due to the upcoming retirement of Prof. Alberto.

8 Third Party Funds

8.1 Newly Approved Third-Party Funding of URPP Project Leaders

SNSF - Divisions I to III

- Prof. Jürg Osterwalder, Model systems for single-atom catalysts and 2D-confined catalysis studied by in situ surface science methods, SNSF Grant 200020 200303, 04.2021 – 07.2022, CHF 365'644.
- Prof. Sandra Luber, Forefront approaches for modelling of compounds and their application to water reduction catalysis, SNSF Project 204265, 10.2021 – 09.2025, CHF 620'000.

Others

- CSC Scholarship for Zeyi Zhang from 11.2021 – 10.2025 (project leader: G. R. Patzke), PhD salary paid to Z. Zhang.
- CSC Scholarship Han Zhao from 11.2021 – 10.2025 (project leader: G. R. Patzke), PhD salary paid to H. Zhao.

8.2 Ongoing Third-Party Funding of URPP Project Leaders

SNSF - Divisions I to III

- Prof. Roger Alberto, Solar Light-driven Homogeneous Catalysis for Greener Industrial Processes with H₂ as Energy Source and CO₂ as C1 Building Block, 02.2017 – 01.2021, CHF 346'189.
- Prof. Peter Hamm, 200020B 188694/1 (Extension: Ultrafast Vibrational Spectroscopy of Allosteric Proteins), 01.2020 – 12.2022, CHF 773'577.
- Prof. Jürg Osterwalder, Surface Physics with Single-Layer Materials and Molecular Layers, SNSF Grant 200020 172641, 04.2017 – 03.2021, CHF 839'027.
- Prof. Karl-Heinz Ernst, Advanced chiral surface systems, 10.2018 – 09.2022, CHF 530'768.
- Dr. Andreas Borgschulte, Ultra-High Pressure Hydride X-ray Photoelectron Spectroscopy, 172662, 03.2018 – 02.2022, CHF 463'400.
- Prof. Sandra Luber (SNSF Professorship), In Silico Investigation and Design of Bio-inspired Catalysts for Water Splitting, 03.2017 – 08.2021, CHF 1.6 Mio.

SNSF - Division IV

- Prof. Peter Hamm, NCCR Molecular Ultrafast Science and Technology (MUST) Phase III, 06.2018 – 06.2022, CHF 720'000.
- Prof. Jürg Osterwalder, NCCR Molecular Ultrafast Science and Technology (MUST), Phase III Project "Ultrafast Structural and Electron Dynamics in Surfaces", 07.2018 – 06.2022, CHF 350'000.

Others

- CSC for Scholarship Hang Chen from 02.2019 – 02.2023 (project leader: G. R. Patzke), PhD salary paid to H. Chen.
- CSC Fellowship for Zhenbin Wang, 10.2019 – 09.2023 (project leader: S.D. Tilley), CHF 100'800.
- Prof. David Tilley, Photoelectrochemical Synthesis of Hydrogen Combined with Water Desalination, PERA Complexity Project, 09.2020 – 08.2021, CHF 110'384.
- Prof. Jürg Hutter, Grant from Swiss National Supercomputing Center, 2019 – 2021, ca. 8.4 Mio core hours per year.
- Dr. Andreas Borgschulte, Joined Empa-PSI project Synfuel, ETH Board, 01.2021 – 12.2023, 6 Mio. CHF (Borgschulte group ca. CHF 400'000), Empa).
- Prof. Sandra Luber, Two grants from Swiss National Supercomputing Center, until 2023.
- Prof. Sandra Luber, Grant from Platform for advanced computing in Europe.

8.3 Newly Funded Projects within Profit-Center (PC) of the URPP

none

8.4 Ongoing Projects within Profit-Center (PC) of the URPP

- Prof. Greta R. Patzke, Forschungskredit to Devi Prasad A S, 01.2021 – 09.2021, CHF 43'160.
- Prof. David Tilley, Photoelectrochemical Synthesis of Hydrogen and Value-Added Chemicals for a Sustainable Chemical Industry, SNF Grant 200020_184737, 09.2019 – 08.2023, CHF 900'000.
- Prof. David Tilley, Forschungskredit to Dr. Wooseok Yang, 09.2019 – 08.2021, CHF 73'515.

9 Specific Tasks and Problems

During the reporting year, LightChEC research and events were influenced by the ongoing pandemic and by the move of many groups of the consortium to the new chemistry buildings on the Irchel campus. While the latter delayed experimental research for a short time, it also rewards the respective groups with new laboratories and instrumentation now and in the future.

Patzke: The move of our group in December 2021 to the new UZI-5 building went smoothly with a lot of technical and administrative support. After a short time in the new lab environment, we already benefited from the excellent infrastructure and the improved communication options for our group in the new setting with no more distribution of our labs over several buildings and floors.

In the coming year, our group would like to connect the URPP LightChEC more strongly to the prominent UZH sustainability strategies.

Tilley: The problem of our group's access to XPS is temporarily solved, as we have user access on an old machine at EMPA. It is so old that it cannot be repaired once it breaks, and the scientists at EMPA expect this to happen at any time. Once we lose access to this, it is the same problem as before: a big bottleneck in our research.