Editorial

The Swiss Energy Strategy 2050 has set a new pace for Switzerland on the road to efficient and renewable energy. To make a carbon-neutral future our next reality, joint efforts of economy, science and society are required. Large-scale decarbonization has the potential to revolutionize our work environments and will also be a source of continuous education for *everyone* involved in the development and implementation of the required technological solutions. While many of them are already available on a larger scale, fundamental aspects of energy materials remain unresolved, especially in catalysis. We have thus devoted this issue of CHIMIA to clean H_2 production and CO_2 reduction, which are often discussed under the umbrella of 'artificial photosynthesis'. Chemistry holds the key to unleash water and sunlight as our boundless sources for virtually unlimited access to renewable H_2. Likewise, the selective reduction of CO_2 after its successful removal from the air is at the forefront of electrochemical and molecular research. This special issue provides fascinating highlights of Swiss research groups which tackle these internationally competitive 'hotspots' of sustainable energy carriers from all angles. Our article selection brings together a wide range of technological, molecular design, physico-chemical and theoretical approaches. The integration of these complementary research competences is essential to make best use of the earth's element resources for catalysts that are affordable, long-lived and efficient.

To start, the article *Hydrogen Storage by Reduction of CO_2 to Synthetic Hydrocarbons* by ***Andreas Züttel and coworkers*** sets the stage for techno-economic aspects with general insight into the advantages of H_2 storage in hydrocarbons, and proceeds to the mechanistic details of CO_2 methanation with nanoscale catalysts. Challenges and progress in electrochemical CO_2 reduction are highlighted, and concise economic perspectives for the different approaches to CO_2 conversion round off the overview. Next, ***Peter Broekmann and coworkers*** lead us right into the arena of electrochemical CO_2 reduction with their new results that tell us to *Unwrap Them First: Operando Potential-Induced Activation Is Required when Using PVP-Capped Ag Nanocubes as Catalysts of CO_2 Electroreduction*. The international author team shows how to turn an as-synthesized nanocatalyst with tuned morphology into a long-lived active material with a single, elegant *operando* activation step. ***Kevin Sivula and Arvindh Sekar*** shed (solar) light on the great potential of *Organic Semiconductors as Photoanodes for Solar-Driven Photoelectrochemical Fuel Production*. Here we are introduced to the emerging discoveries of organic-based light harvesters for water-splitting setups as highly tunable molecular and carbon-based alternatives to metal oxide components. Then we move further into the heart of artificial photosynthesis with ***the team of Roger Alberto*** who present their progress on *Cobalt Complexes of Polypyridyl Ligands for the Photocatalytic Hydrogen Evolution Reaction*. Starting from profound insight into the mechanisms of new H_2 evolution catalysts and their optimal electron relays and donors, the team masters the leap from fundamental homogeneous molecular processes to their application-oriented heterogeneous immobilization. We then learn more *About Control: Kinetics in Molecule Based Photochemical Water Reduction Investigated by Transient IR Spectroscopy* from ***Peter Hamm and Kerstin T. Oppelt***, namely what really happens when such molecular water reduction catalysts are at work on oxide surfaces. The power of transient spectroscopy delivers the indispensable mechanistic insight into the translation of molecular catalyst design in solution into their optimal operation in surface-bound systems. Proceeding from physico-chemical to theoretical aspects of water splitting, the issue gives an outlook on the enormous modeling possibilities for understanding and engineering water splitting catalysts. ***Sandra Luber and her team*** make impressively clear *How ab initio Molecular Dynamics can Change the Understanding of Transition Metal Catalysed Water Oxidation*. This hands-on review of their work on representative ruthenium-based molecular water oxidation catalysts demonstrates great progress in understanding key solvent environment effects and mechanistic aspects of O-O bond formation with advanced DFT-MD methods. These insights are furthermore vital for informed ligand tuning of complexes to optimize their water splitting efficiency. Finally, the molecular realm is complemented with the robustness and tuning options of heterogeneous systems by ***Ulrich Aschauer and his team***, who discuss the *Surface Chemistry of Perovskite Oxynitride Photocatalysts* - (from) *a Computational Perspective*. This unique direct insight into the surface processes of highly versatile mixed-anion perovskite materials during oxygen evolution is essential to leverage their full potential for photoelectrochemical applications.

This issue of CHIMIA offers a fascinating journey into the diverse and forefront dimensions of Swiss research on green H_2 production and CO_2 conversion, which is further strengthened by larger networks, such as the NCCR *Catalysis* or the URPP *Light to Chemical Energy Conversion* (University of Zurich). We hope that this overview will be inspirational for both young researchers and seasoned experts in the field to join the ongoing journey to protect our climate with 'Better Living Through Chemistry'.

Prof. Greta R. Patzke
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Credits for the cover illustration (clockwise): center, circular economy with H_2/CO_2 (Andreas Züttel, EPFL), top left: defective oxynitride surface (Ulrich Aschauer, University of Berne), top right: scheme of surface-immobilized water reduction catalysts and photosensitizers (Peter Hamm & Kerstin T. Oppelt, University of Zurich), middle right: model of CO_2 reduction pathways on a catalyst surface (Andreas Züttel, EPFL), bottom right: organic semiconductor for solar-driven water splitting (Kevin Sivula, EPFL), bottom left: CO_2 reduction with activated Ag nanocubes (Peter Broekmann, University of Bern), middle left: free energy surface of a molecular water oxidation catalyst (Sandra Luber & Rangsiman Ketkaew, University of Zurich).

The Editorial Board of CHIMIA warmly thanks Prof. Greta R. Patzke for planning this issue on 'H_2 Production and CO_2 Conversion: Insights and Progress' highlighting the vital research relating to sustainable energy technology for the future.