Summary

Mitigating climate change is imperative to prevent its severe impacts on human health, the environment, and the global economy. The Glasgow Climate Pact (2021) marked a pivotal step in addressing these challenges. Hydrogen has emerged as a promising alternative energy source, offering the advantage of producing water as its sole byproduct without emitting pollutants such as particulate matter or greenhouse gases like CO_2. Chapter 1 illustrated various methods which have been developed for hydrogen production, often categorized using a "rainbow code" to distinguish between different pathways. Among the possible pathways, conventional methods, such as steam methane reforming (grey hydrogen) and coal gasification (brown hydrogen), rely heavily on fossil fuels, resulting in significant CO_2 emissions. Recent advancements, such as carbon capture and storage technologies, have enabled the production of blue hydrogen (*i.e.* H_2 produced via Steam Methane Reforming or Auto Thermal Reforming, with by-product carbon dioxide captured and stored), reducing CO_2 emissions in industrial processes. Among these strategies, green hydrogen is one of the most environmentally friendly approaches, utilizing renewable electricity to drive water-splitting reactions. Despite its potential, green hydrogen production accounted for only 0.1% of the global energy demand in 2023, according to the International Energy Agency. Addressing this shortfall requires the development of innovative solutions for industrial-scale implementation. Available technologies for electrochemical water splitting to produce green hydrogen include proton exchange membrane (PEM) electrolysers and anion exchange membrane (AEM) electrolysers. PEM electrolysers operate under acidic conditions and require catalysts with exceptional activity and stability, often relying on noble metals. In contrast, AEM electrolyser technology has progressed toward using non-noble metals, particularly for the oxygen evolution reaction (OER). Due to the collaboration with Ohmium Internation, Inc. regarding OER in acidic media and the Inorganic Chemistry Department of the University of Vienna with Austrian Institute of Technology (AIT) regarding OER in alkaline electrolyte, the materials' selection was carried out to satisfy the needs of each partner. In particular, computational studies have shown that among the screened materials, transition metal oxides, perovskites, chalcogenides, phosphides, and borides have been reported as most promising materials. In particular as reported in Chapter 2, the antimonates represented a class of materials with features that could have overlapped the industrial needs of our collaboration with Ohmium company. For this reason, the selection fell on cobalt antimonate. Regarding the development on novel electrocatalysts for alkaline OER, the selection was made towards the Ni metal-organic framework (Ni-MOF) due to the expertise of the researchers at the University of Vienna on MOF synthesis and development.

In Chapter 3 $CoSb_2O_6$ was studied towards acidic OER. In particular, the study aimed to investigate the effects of calcination time and temperature during the synthesis of $CoSb_2O_6$. The best conditions that allowed to obtain the highest amount of $CoSb_2O_6$ (87%), which posed the basis for subsequent scale up of electrode's sizes. In Chapter 4, $CoSb_2O_6$ has been deposited onto a fluorine-doped tin oxide (FTO) supporting material in order to evaluate the O_2 production and the Faradaic Efficiency (FE). $CoSb_2O_6$ has reported a FE higher than 99%, resulting a selective catalyst for O_2 production. Moreover, to improve catalytic performance, the Pt introduction was explored. Different methods have been exploited to introduce different amounts of Pt inside $CoSb_2O_6$. The samples with the lowest amount of Pt (0.16%) have reported the highest improvement in terms of overpotential reduction. In Chapter 5, the development of Ni-MOF based materials is displayed. Such study was

conducted at both the University of Vienna and AIT facilities and was developed starting from the Ni-MOF synthetized by using a biphenyl ligand and tested it in alkaline solution towards OER. Afterwards, the ligand was exchanged with a noble-metal-doped bipyridine ones. The study aimed to evaluate the stability after a 2-hour lasting chronopotentiometric test and the activity of these materials. The best performance was shown by Ni-MOF(Pt-BPy)/NF with an overpotential of 267 mV to reach a current density of 10 mA cm^{-2}. In Chapter 6 the conclusions and the outcome of this work are summarized.