In the first part of the thesis, a series of first row transition metal complexes have been synthesized in order to study their mechanism and efficiency as a hydrogen gas (H$_2$) evolution catalyst. The H$_2$ produced can served as an alternative clean fuel to tackle the issue on climate change. A comprehensive characterisation of the electrochemical and spectroscopic properties of these complexes has been performed. The efficiency and the mechanism of these materials and complexes have been studied.

In the second part of the thesis, the surface modification on oxide-derived copper (OD-Cu) and its influence on the products distribution of CO$_2$ reduction on copper (Cu) were investigated. It was found that the majority of the crystal facets in the polycrystalline OD-Cu can dictate the major products formed and can greatly influence the overpotentials for CO$_2$ reduction.