Publishable executive summary

Within the FCAnode project, all workpackages performed with the objectives to find Proton Exchange Membrane Fuel Cell (PEMFC) anode catalysts of reduced cost and competitive performance to the current state-of-the-art Pt and PtRu catalysts.

The novelty of this project has been the full development of novel catalyst nanoparticles for fuel cell applications from theoretical design to the final operating membrane electrode assembly. For the first time, theoretical studies have been associated to experimental studies for the development of novel catalyst nanoparticles for fuel cell applications. A loop between theoretical calculations and experimental characterisations has been created and input coming from the experimental results into the theoretical calculations has taken place within the project. This novel methodology has been demonstrated throughout this project to be very powerful for the development of novel catalyst nanoparticles for fuel cell applications. This is, to our opinion, the best structure for projects aimed at searching for new promising catalytic systems for fuel cells. Due to the multidisciplinary approach, this novel powerful methodology can hardly be performed at national level and needs to be performed at European level in order to assemble the expertise in the various fields of investigation.

Modelling exercices through Density Functional Theory (DFT) calculations have been initially conducted in the search for potential candidates for the Hydrogen Oxidation Reaction (HOR) at the PEMFC anode. Critical bond energies and activation barriers of the processes have been calculated and trends in reactivities for bimetallic and alloy species have been produced. These trends in reactivities have been used for the production of a “library” of potential novel materials.
Selected systems from the “library” have then been synthesised as model systems and a wide range of compositions have been investigated by combinatorial screening.
The resultant most promising systems have been synthesised as carbon-supported catalyst nanoparticles and characterised by a variety of ex-situ and in-situ microstructural analysis techniques. They must show sufficiently high density of hydrogen oxidation to make them realistic competitors to current platinum-based catalysts, while remaining stable in the humidified fuel cell environment at potentials of up to +400 mV, and exhibiting the necessary tolerance to CO. These properties have been experimentally investigated by adsorption, electrochemical and single cell testing studies following an initial benchmarking study on state-of-the-art Pt and PtRu catalysts. An insight into the fundamental understanding of the CO tolerance issue has been obtained comparing the CO adsorption/desorption properties of the Pt and PtRu benchmarking catalysts. The CO tolerance properties of some of the most promising systems have then been further investigated. The performance of the most promising systems for HOR and their stability in acidic media have been assessed using electrochemical techniques. Membrane electrode assemblies have been produced using the selected anode catalysts and their behaviour has been assessed within the single cell environment in order to be closer to real fuel cell working conditions. The potential for large-scale production of the newly developed most promising carbon-supported nanoparticles by practical industrial methods has been also investigated. In addition, studies at higher temperatures than the current PEMFC operating range have

been carried out, since the focus is now on higher temperature membranes for increased performance.

The main project successes are summarised below:

- The production of a “library” of potential novel materials
  Density Functional Theory calculations have identified potential catalysts for HOR and combinatorial fast screening has been performed on these potential systems regarding hydrogen oxidation and CO tolerance.
- The development of advanced platinum-based catalyst standards
  State-of-the-art platinum-based catalyst standards have been developed; while benchmarking for the adsorption, electrochemical and single cell testing programmes has been performed.
- The identification of optimum synthetic routes and optimum supports for the production of novel supported PEM fuel cell anode catalyst
- The development of novel systems with lower noble metal content
  Several systems with lower noble metal content and consequently lower cost and several entirely non-noble systems have been synthesised and fully characterised within the project.

As an outcome of the project, three systems have been identified as the most promising systems with potential for reduced noble metal content or cost. Two systems have been identified as the most promising systems with zero noble metal content. Another system presenting a very high CO tolerance has been also investigated in detail. A full characterisation of these systems in terms of optimal composition, optimal synthesis method, CO tolerance, electrochemical behaviour and single cell testing has been performed within the project. In terms of cost, the two systems with zero noble metal content appear as the most promising systems, since it does not content any noble metal. Their electrocatalytic activities are however much lower than that of the systems with reduced noble metal content. In terms of cost and electrocatalytic activity, the systems with reduced noble metal content present properties, which make them viable competitors to the current state-of-the-art Pt and PtRu catalyst. Five patent applications have been filed in relation with the most promising systems determined within this project. This is the reason for not disclosing proprietary information on the identified catalyst systems. In addition, more than twenty publications in peer-reviewed scientific journals have originated from the project.

As a conclusion, a novel powerful and very promising methodology based on the combination of theoretical and experimental studies has been used within this project for the development of novel catalyst nanoparticles for fuel cell applications. Viable competitors to the current state-of-the-art Pt and PtRu catalysts having a reduced noble metal content have been determined within the FCAnode project. This has led to a number of peer-reviewed publications in scientific journals from the consortium and to the filing of patent applications for the most promising systems. These results make, in our opinion, FCAnode a successful project.