Publishable Summary

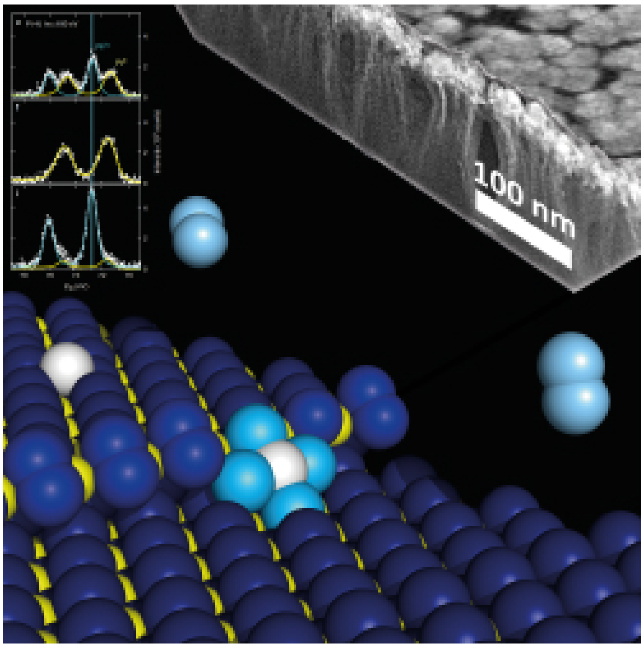
Overview of project context and objectives

The chipCAT project (FP7 GA no. 310191) was established by research groups with successful record in fundamental research of catalysts for proton exchange membrane fuel cells (PEMFC) and partners from related industrial fields. Our principal aim was to continue the promising explorations of the missing fundamental knowledge in catalysis and, at the same time, utilize this in knowledge-based development of technologies for cheaper, more durable and more mobile industrial-level fuel cells.

The motivation for our work was to contribute, with our expert knowledge and facilities, to making substantially more affordable proton-exchange membrane fuel cells, which were staying at high prices owing to the amounts of Platinum, expensive catalyst production and FC assembly and limited lifetime of the catalysts. As the envisaged new thin-film catalyst technology would be compatible with integrated circuit devices in Silicon wafer chips, we proposed to make an attempt at application of the catalyst films in making a prototype of and on-chip microfluidic fuel cell.

These were the principal objectives:

- By way of model experimental and theoretical (computational) physics uncover the precise mechanisms behind the function of the Platinum-based low-noble metal content catalysts, especially in combination with reducible oxides;
- Transfer of the patented low-noble metal content catalyst preparation method from model to practicable industrial scale;
- Explore a selection of other low-Platinum or precious metal-free catalysts for their suitability for deposition by the developed physical method and in planar geometry.



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- Develop a physical thin-film catalyst preparation method compatible with the standard planar processes in semiconductor device industry;
- Develop a complete functional prototype of a microfluidic PEMFC device;

The consortium Coordinated by the surface physics group at Charles University in Prague (CUP) engaged computational modelling, model and applied experiments and technology and device development to achieve the objectives.

Work performed during the project

Fundamental materials research

The studied materials required gaining extra fundamental knowledge in of structure, electronics and physico-chemical activity with respect to hydrogen, oxygen, carbon monoxide, small hydrocarbons and similar. The materials, modelled on one hand in computational simulations (prof. K. Neyman, University of Barcelona, Spain, prof. S. Fabris, National Research Council, Italy) and fabricated in model systems for physical analyses (prof. J. Libuda, Friedrich-Alexander University in Erlangen-Nuremberg, Germany), were Platinum, Palladium, Gold, Cobalt, Nickel and other elemental metals pristine or alloyed, in the form of metallic or metal-oxide nanoparticles or even atomically dispersed on top crystallites or thin films of CeO2 (ceria), CeSnO2 (mixed cerium-tin oxide) and WO3 (tungsten oxide).

The largest amount of work was devoted to simulations and measurement of Platinum-ceria and related materials, but the elemetal metals and alloys in nanoparticular form received their share in model studies as well. The chief computational methods employed were DTF, DFT+U and molecular dynamics, while the main analytical methods were x-ray photoemission-based and infra-red absorption-based spectroscopies (XPS, IRAS), atomically-resolved scanning tunneling microscopy (STM) and high-resolution TEM.

Applied research of materials

Indeed, while the quality of the heterogeneous catalysts was clear from model studies, the applied work focused on recipes for catalyst deposition in large-active-surface structures (prof. V. Matolin, Charles University in Prague, Czech R.). The catalytic materials (and candidates) were in the form of thin films deposited on various substrates ranging from flat silicon and graphite to highly porous graphitic materials like carbon nanotubes and nanoparticles, CN (carbon nitride). Methods for thin film deposition were magnetron deposition and atomic layer/chemical vapour deposition, sometimes on substrates obtained by “wet” chemical processes. Several materials such as WC and WCO (tungsten carbide and oxycarbide) were studied as candidates for Platinum-free catalysis (prof. S. Bourgeois and prof. B. Domenichini, University of Burgundy in Dijon, France).

The analytical methods used here were again photoemission methods and HRTEM, but also others such as SEM, electro-chemical AFM, chemical micro-reactors with electrochemical cycling, some of them tied to infrared spectroscopy.

Technological development

The titular on-chip micro-fuel cells development required us to test and prove several key enabling ideas: the microchannel design, the electrodes’ deposition and lithography, the sealing with a proton-exchange membrane, interfacing with fluidic and electronic testing facility, complete testing. These tasks were all carried out by ThunderNIL s.r.l., an SME in Trieste, Italy, in collaboration with the Coordinator and L.E.T. optomechanika Praha s.r.o, another SME in Prague, Czech R. The development of a new family of nanocatalysts was based on the fundamental and applied work, but required also robust testing that followed industrial standard protocols and aimed to meet industry targets for performance. The project used the expertise and testing facilities of SolviCore GmbH & Co. KG in Hanau to test several dozens of sample catalysts in membrane assemblies. During the project the Coordinator developed its own testing facility, so that the testing load gradually shifted there.

Results proposed and achieved

The proposed final results were:

- By way of model experimental and theoretical (computational) physics uncover the precise mechanisms behind the function of the Platinum-based low-noble metal content catalysts, especially in combination with reducible oxides;
- Transfer of the patented low-noble metal content catalyst preparation method from model to practicable industrial scale;
- Explore a selection of other low-Platinum or precious metal-free catalysts for their suitability for deposition by the developed physical method and in planar geometry.
- Develop a physical thin-film catalyst preparation method compatible with the standard planar processes in semiconductor device industry;
- Develop a complete functional prototype of a microfluidic PEMFC device;

This was the 3rd and last period of the project and all these objectives were achieved.

All the theoretical and experimental work of Work Packages 2 through 5 was successfully applied in the standard proton-exchange membrane fuel cell assemblies tested in WP6. The research work also resulted in 71 articles published in peer-review journals, 30 of them collaborative ones including some in Angewandte Chemie Int'l Ed., Nature Materials and Nature Communications. The nanocatalyst films developed and the fuel cell testing stations - electronic and gas flow assemblies for testing individual membrane assemblies - have been marketed through LEANCAT Ltd, a commercial venture newly established between the Coordinator and a venture capital investor. Thorough durability tests of fuel cell catalysts are time-consuming (ca. 1 complete test per week) and the private capital facilitated to eliminate this bottleneck by allowing the construction of a 10-station testing center. The convincing performance of both, catalysts and the testing stations, resulted in transforming the commercial project into an entity, the LEANCAT Ltd, which now offers the nanocatalyst technology and fuel cell testing as services and testing stations as a high-tech product.

The key enabling ideas for PEM micro-fuel cells were developed and tested and prototypes of these on-chip devices were successfully tested in WP 7. The challenges were overcome and resulted in on-chip microchannel devices with tiny but stable power output. This technology has been, hence, developed into working laboratory prototype representing Technology Readiness level 3 or 4.

Contacts

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