Challenges and Directions in Electrocatalyst Research for PEMFCs

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A present challenge in the development of polymer electrolyte fuel cells is to achieve sufficiently high power densities >1W/cm² at voltages >0.8 V. Under such operation conditions the ratio of electrical power (P_{el}) and co-generated heat (P_{th}) is $P_{el}/P_{th}>2$. Thus, on one hand a higher energy conversion efficiency of the fuel cells would be achieved; on the other hand, the heat management of the fuel cell stack and system requires a less complicated design and hence decrease costs. In order to tackle these targets the following aspects need further development:

- In H_2/O_2-cells the catalyst of the cathode has to be improved. In alcohol/ O_2-cells the anode and cathode reaction rates have to be enhanced;
- Supports other than carbon based materials should be taken into account;
- The overall resistance of the catalyst layer needs to be decreased with respect to the electron and proton conductivity;
- The mass transport in the catalyst layer has to be optimized in order to limit transport problems of reactants and products at high current densities.

In catalyst development nowadays it is possible to identify promising candidates using density functional theory (DFT), as was shown for example by Nørskov et al.[1,2] Especially non-noble, possibly bimetallic materials should be considered. For such materials the electrocatalytic activity can be influenced by alloy formation.[1] It is known that the activity of electrocatalysts is furthermore determined by particle size.[3, 4 , 5] Consequently a major aspect will be to identify the optimal particle size and particle distribution in order to achieve the maximum utilization of catalyst material.

Also, novel non-carbon based support materials with higher corrosion stability and improved conductivity can be of importance. For example, ruthenium oxide (RuO_x $(H_2O)_y$) was shown to be a promising material because it provides both, electron and proton conductivity.[6] This helps to increase the utilization of the catalyst. Shortly summarized, in addition to the obvious “quest” for novel catalyst material, we need to understand the major factors that influence the specific activity of a catalyst material: Among these, we have to clarify how the interactions of the catalyst with the support material determine reactivity. This includes further an understanding of individual particle reactivity. Furthermore, we have to understand the structure- and size reactivity correlation in greater detail.

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