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Conversion of hydrogen on alloys and inorganic compounds

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The Platinum metals are the only real good materials for producing hydrogen by electrolysis and for converting it in the low temperature PEM cells. The production of platinum only amounts to some 190 ton/year [1] and can thus easily be a severe show stopper for a future hydrogen economy [2]. There is therefore a strong demand for finding new cheap and more effective materials. This naturally involves understanding the problems with current systems.

The dissociation of Hydrogen on conventional Platinum metal anode electrode on Proton Exchange membrane Fuel Cells (PEMFC) are known to be strongly inhibited by adsorption of for instance CO. This effect has been investigated in detail both on Pt [3] and Pt/Ru [4] anode by using CO exchange experiments on commercial electrode materials. This method allows for determination of the CO desorption rate under operation condition and a CO pressure controlling the CO coverage. The results show that the Ligand effect, i.e. that the strength of the CO bonding prevails in importance over the bi-functional effect under realistic operation conditions. This despite the fact that the CO desorption rate on the nanoparticles constituting the anode materials on the commercial electrodes shows a substantial lower exchange rate than on a Pt(111) model surface [5]. The observation is explained by a confinement effect on the nanoparticles where the packing of the CO must be quantized. These results are used to search for new alloys by a parallel screening approach where the search for catalyst that are good at dissociating hydrogen in the presence of CO and water are performed in a combined UHV-high pressure cell equipment [6].

The electrochemical hydrogen evolution process whereby protons and electrons are combined into molecular hydrogen is also catalyzed most effectively by the Pt group metals [7]. This can be understood in terms of general trends in reactivity of Hydrogen [8] and the criterion that

$\Delta G_H^0 \cong 0$ for the process seems to be an essential demand. Hydrogenases and nitrogenases are also effective catalysts for the hydrogen evolution process, even though the catalytically active site of these enzymes contains the much less noble metals Fe, Ni, and Mo, and the nitrogenase active site contains S. Based on this criterion and especially by this biomimetic inspiration from nature has led to investigation of MoS₂ nanoparticles as a new material for hydrogen evolution [9]. Indeed, our experiments show that MoS₂/graphite is a quite reasonable material for hydrogen evolution with an overpotential of the order 0.1-0.2 V. This is in excellent agreement with the predictions from theory, and it suggests that we can begin searching for new catalytic materials using quantum chemical methods. The MoS₂ nanoparticles supported on graphite may be an example of a new class of electrode materials,

and there are good possibilities for further optimization.

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