Methanol Electro-oxidation Mechanism on Rare Metal Surfaces: A DFT Study

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ABSTRACT

Direct Methanol Fuel Cells (DMFCs) have attracted many researchers in the past decades due to its promising properties that can be used for several applications. Development of active electrocatalysts for both anode and cathode is needed for better DMFCs. In the anode, efforts are being concentrated on the design of highly active catalysts for methanol electro-oxidation reaction (MOR)¹³. Even though the Pt-Ru alloy is known as a good catalyst for MOR, further improvement of its catalytic activity using an additional third metal is still being considered²⁴. Using Density Functional Theory (DFT), we clarify the role of Ru and Mo in the PtRuMo catalyst system for possible promising catalysts. A model for simulating MOR in which we take into account the H₂O and hydronium ion H₃O⁺ as coadsorbed species was used. We also introduce possible way to increase the coverage of (O)ads and (OH)ads oxygenated species which is believed to be useful for completing MOR⁵, i.e., by the formation of hydroperoxo (OOH) intermediate since it weakens O-O bond on Pt surfaces⁶⁷. Our results show that the presence of coadsorbed species weakens the interaction between surfaces and MOR intermediates. Additional Mo metal in PtRuMo catalyst systems responsible for increasing (O)ads and (OH)ads coverage due to its ability to capture (O)ads and (O₂)ads, while Ru catalyzed the OOH breaking to form (O)ads and (OH)ads in this mechanism. Then, the increase of (OH)ads coverage on the surface weakens the Pt-CO bond strength which mean that it becomes easier to remove CO from surface. More details will be explained in the conference.

Keywords: DMFCs, MOR, coadsorbed species, oxygenated species

References