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The Double-edged Impact of Platinum Nano-Deposits on the Durability of Polymer Electrolyte Membranes — A Theoretical Study[1]

MOHAMMAD JAVAD ESLAMIBIDGOLI, PIERRE-ÉRIC ALIX MELCHY, ATA ROUDGAR, MICHAEL H. EIKERLING, Simon Fraser Univ — The attack of oxygen radicals is one of the main sources of chemical degradation in the polymer electrolyte membranes (PEM) of polymer electrolyte fuel cells. In this context, Pt in the membrane (PITM) that originates from Pt degradation in the cathode catalyst layer plays a double-edged role: surface reactions at PITM could facilitate the formation or quenching of radicals. The balance of these processes depends on the local electrochemical conditions, determined by thermodynamic parameters and local composition of the PEM. The objective of this work is to explore the equilibrium and kinetics of radical reactions at PITM as a function of local PEM conditions. We first determine the potential distribution of PITM based on a continuum model of crossover of reactant gases coupled with their local electrochemical reactions at Pt. Secondly, we determine the surface state of Pt for the given local potential using relevant experimental data and kinetic models of surface reactions at Pt [1, 2]. Lastly, we use this information as input for *ab initio* calculations at the DFT level of specific processes involved in the radical balance at the Pt | water interface.

[1] M. Wakisaka et al. Langmuir, 25, (2009)
[2] S. G. Rinaldo et al. submitted to Nat. Mater. (2013)

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