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Effect of carbon support on catalytic efficiency and durability in fuel cells CECILE MALARDIER-JUGROOT, MICHAEL GROVES, DEBORAH DURBIN, MANISH JUGROOT, Royal Military College of Canada — New nanomaterials already play a key role in several emerging technologies. For instance, in fuel cell technology, catalytic efficiency can be greatly enhanced due to the high surface area of nanomaterials. Improving the durability and efficiency of a platinum catalyst is an important step in increasing its utility when incorporated as the anode or cathode of a proton exchange membrane fuel cell (PEMFC). The authors have shown using Density Functional Theory methods [1] that doping the carbon support of the Pt catalyst can increase the durability and efficiency of the catalyst. This paper will present the effect of doping of the carbon support on the complete reaction path of the Oxygen Reduction Reaction using *ab initio* structural methods as well as a complete *ab initio* molecular dynamics characterization of the reaction. In addition, the electronic structure of the carbon support was shown to improve the metal/CO interaction for the development of a membrane to prevent catalyst poisoning [2]. The paper will also emphasize the effect of the solvent, which is experimentally shown to be crucial. [1] M. Groves, A. Chan, C. Malardier-Jugroot and M. Jugroot, *Chem. Phys. Letters*, 481(4-6), 214-219, 2009 [2] D. Durbin and C. Malardier-Jugroot, *J. Phys. Chem. C*, 115 (3), 808–815, 2011

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