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Influence of water on the reaction path of the oxygen reduction reaction in fuel cells CECILE MALARDIER-JUGROOT, MICHAEL GROVES, MANISH JUGROOT, Royal Military College of Canada — The development of fuel cell technology has been limited in part due to the cost of the catalyst used in the cell and the rate limiting oxygen reduction reaction. We will present a molecular modelling study focus toward the prediction of improved durability and catalytic efficiency of the Platinum catalyst using doped graphene and doped single walled carbon nanotube surface. The most promising carbon supports - active centre systems were then studied in the gas phase and with explicit water molecules to model the oxygen reduction reaction and tailor the catalytic centres to improve the efficiency of this reaction while reducing the probability of occurrence of side reactions. Two major conclusions have been drawn from this analysis of the oxygen reduction reaction with and without water present. The doping of the carbon surface leads to a stronger platinum-surface interaction and does help the breaking of the oxygen-oxygen bond. These two are interrelated since the stronger surface-platinum bond allows for the same orbitals to interact with the oxygen-oxygen orbital. In addition, the dopants could make the surfaces more polar thus retaining water which might help catalyze the reaction, this property could be very promising to increase the effectiveness of fuel cell cathodes.

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