

Behavior of Ionic Species in Sulfonated PEI Using DFT Simulations: A Study to Determine Ionic Conductivity.

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ABSTRACT

Compared with internal combustion engines, proton exchange fuel cells (PEMFC) are able to operate without polluting emissions. Increasing the operating temperature of the fuel cell above 100 °C is one of the major objectives in this field as it would facilitate the commercial development of electric vehicles powered by fuel cells. To achieve this objective, it is important to develop new types of membranes to replace Nafion. The poly (ether imide) sulfonated are presented as a new alternative in order to use as an electrolyte in PEMFC. In this work, DFT theory has been used to study the interaction between ionic species charged of hydrogen as hydroxyl ((OH)-) or hydronium ((H₃O)+) and sulfonated poly(ether imide). The analysis of molecular reactivity through frontier MO (HOMO and LUMO) allows to determine the mechanism of ionic conductivity which takes place over the polymeric membrane. This study is addressed to improve the efficient of PEM fuel cells.

Keywords: Fuel cell, conductivity, ionic species

