



**Wolfson Department of Chemical Engineering Special Seminar**  
**Lecture Hall 6, Wolfson Department of Chemical Engineering,**  
**Thursday January 4<sup>th</sup> at 15:30**

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**Characterization of Anion Exchange Ionomers for Fuel Cell Applications**

Anion exchange membrane fuel cells (AEMFCs) have recently received increasing attention since they allow for the use of non-precious metal catalysts, which can dramatically reduce the cost of fuel cell devices. Anion exchange ionomers (AEIs) are critical to the AEMFCs, as they provide the electrodes with hydroxide conductivity, enabling maximization of the catalyst utilization in the fuel cell device. In AEMFC, water is a reactant in the cathode electrode and a product in the anode electrode, which results in the water gradient through the anion exchange membrane (AEM). Without water in the membrane, AEM is unable to conduct ions, hence water interaction with the ionomeric materials is critical. In spite of this, to our best knowledge, there are no research studies on water-ionomer interaction for anion conducting ionomers. In order to increase the understanding of the water-ionomer interaction, thin films of different anion conducting ionomeric materials were prepared and characterized. This work summarizes the findings, which we believe will provide first useful insights into the water-ionomer interaction.

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**Molecular dynamics simulations of QA-OH salts at low hydration**

Anion exchange membrane (AEM) is a core component of anion exchange membrane fuel cell (AEMFC) devices. The degradation of the quaternary ammonium (QA) cations in AEMs is currently a primary concern in this technology. Present experimental and computational work has focused on the stability of various substituted ammonium salts, however stability of AEMFCs do not correlate well with the current studies. Very recently, new studies found that while cation chemistry affects its stability, degradation is mainly related to the hydration level in the cation environment. However, a closer look at this effect is needed in order to better understand the effect of water on the cation stability. In this work we use molecular dynamics (MD) simulations to explore the behavior of three common QA cations with stoichiometric hydroxide concentration and at very low hydration levels. We find that water preferentially solvates the hydroxide anions, and hence when water is present at sufficient amount (more than 4 water molecules per ion pair), stability of the cations increases. However, lower amounts of water result in the formation of isolated molecular clusters and ammonium-hydroxide pairing that presumably leads to degradation of the cation. At low hydration, the composition and size distribution of the clusters is significantly affected by cation chemistry. These observations may provide critical understanding of the barriers to AEMFC stability, and may provide a significant impact to future development of this technology.