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Molecular Design Aspect of Sulfonated Polymers for Direct Methanol Fuel Cells

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Molecular structural features of sulfonated polymers are directly tied to their fuel cell performance [1-3]. Recently, we have demonstrated that percent conducting volume (PCV) correlated well with proton conductivity of multiple, sulfonated polymer electrolytes under fully humidified conditions [4]. The PCV parameter is expressed by the ratio of the volume of the hydrophilic phase to the volume of the hydrated membrane, analogous to the conducting volume of the membrane. PCV was simply calculated from information regarding chemical structure and water uptake using the following equations:

$$PCV = \frac{V_{H_2O} \cdot \lambda}{MVC_{(WET)}}$$

$$MVC_{(WET)} = \sum_i n_i V_i + 18\lambda$$

where V_{H_2O} is the molar volume of water, $18 \text{ cm}^3/\text{mol}$; V_i is the the molar volume [5] associated with the i^{th} structural group appearing n_i times per charges; λ is the hydration number; and $MVC_{(WET)}$ is the molar volume per charge in the hydrated membrane.

Continuing efforts investigating the relationship between molecular structure of sulfonated polymers and fuel cell performance will be discussed in this presentation. In particular, we focus on polymer electrolytes for direct methanol fuel cells. The molecular composition (nanometer length scale) and polymer architecture (sub micrometer length scale) of various sulfonated polymers were considered. For the discussion of molecular composition, polymers have been categorized into polymers containing 1) functional groups, 2) aromatic groups and 3) fluorinated groups. The effect of polymer architecture was investigated by sub-categorizing into 1) homo/alternating, 2) random and 3) graft/block (co)polymers. Combination of length scale variables provides important insight into the design of polymer electrolytes for direct methanol fuel cells. Structure-property relationships and direct methanol fuel cell performance of select sulfonated polymers will be presented in order to support trends between the various parameters investigated.

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