Theoretical Characterization of Sulfonated Poly (ether-imide): A Promising Material for Proton Exchange Membranes in fuel cells.

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Abstract.

Using methods of Density Functional Theory (DFT), Molecular Mechanics and Dynamics, polymers based on Sulfonated Poly (ether-imide) (SPEI) with $(-SO_3H)_n$ (n=1-6) groups were studied to investigate the morphology, properties of proton transport, reactivity and selectivity of these polymers that have important applications in fuel cells. We studied these properties as a function of number of $(-SO_3H)_n$ (n=1-6) groups. We examined the effect of functional group on these properties. The results of geometry optimization in conjunction with ones Raman and Infrared spectroscopy indicated that these polymers have excellent chemical and thermal stability. Besides, in this study, reactivity and selectivity, thermal properties, swelling, water uptake, and molecular interactions were calculated for comparison with other polymers. The comparative study demonstrates that the SPEI exhibit good overall properties for proton exchange membranes in fuel cells.