Design of Biomimetic Proton Wires Based on Helical Peptides: A Quantum Mechanics/Semiempirical Study

ABSTRACT

Over the past two decades, proton transport has been extensively studied because of the many applications to the development of new technological devices. In particular, understanding proton transport permits the design of new materials with desired properties for constructing effective proton exchange membranes (PEM) in fuel cells. Current PEM technology involves expensive perfluorinated membranes that operate under hydrated conditions, for which the proton conductivity is limited by the usually high temperature that fuel cells operate. In addition, due to the toxic and bioaccumulative nature of perfluorinated compounds upon degradation, research has been directed to find alternatives of environmentally friendly proton-conducting materials that operate through a non-solvent mediated mechanism in a wider temperature range.

Studies have shown that histidine-containing materials form proton wires that can potentially be used for proton conduction via GSM. With this, helical peptides with amphiprotic histidine side chains have become promising scaffolds as alternative PEM materials. In our work, three major helical conformations with histidine side chains were investigated as potential proton wire candidates. The structures constructed were modeled using a hybrid computational approach (B3LYP and AM1). The proton wires formed upon hydrogen bonds between ε- and δ-nitrogens were computationally evaluated based on the difference in structural properties and the proton translocation energetics.

Our work offers insight into the fundamental requirements of proton wire formation by modeling non-aqueous proton wires built from biomimetic helical peptides with different characteristics and determining their proton-conducting capabilities.