

Binding, reaction, and activation energies of OH⁻ ions interacting and reacting to some head groups of anion exchange membrane explored via the DFT method

Mirat Karibayev^{1*}, Bauyrzhan Myrzakhmetov², Sandugash Kalybekkyzy², Almagul Mentbayeva^{1, 2}, Yanwei Wang^{1, 3}**

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan.*

²*Laboratory of Advanced Materials and Systems for Energy Storage, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

³*Laboratory of Computational Materials Science for Energy Applications, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: mirat.karibayev@nu.edu.kz, **E-mail: yanwei.wang@nu.edu.kz

The main drawback of Anion Exchange Membranes is related to the chemical instability of cationic head groups and the transportation of hydroxide ions at alkaline conditions and elevated temperatures. At this stage, our research was devoted to understanding the stability and transportation mechanism of hydroxide ions in detail and aiming to reach and keep the performance of AEM for a long time. In this regard, the quantum chemical properties for binding of various hydroxide ion-quaternary ammonium (QA) head group systems were investigated by the DFT method in implicit water to get binding energy. Then, the nucleophilic substitution degradation reaction of various hydroxide ion-QA head group systems were studied by the DFT method at the different hydration levels. Finally, the results of the DFT methods were in line with experimental results on chemical stability and ion exchange capacity.

In this work, we carried out by DFT calculation to get optimized structures of our designed systems, to understand the binding energy of hydroxide ion with six different QA head groups, and degradation reaction of hydroxide ion with two different QA head groups of AEM. Results of binding energies show the following order of the binding strength of OH⁻ ion with six various QA head groups: a) > c) > f) > d) > e) > b), which suggest that the group b) has a high transportation rate of OH⁻ ion via QA head groups of AEM. Considering the comprehensive studies of the Nucleophilic Substitution (SN₂) degradation reactions for QA head groups c) and f), the chemical stability of QA f) is found to be higher than that of QA c), because the activation energy of QA c) is lower than that of QA f), while the reaction energies for QA c) and QA f) are similar at the different hydration level.

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