Designing Highly Efficient OH^- Conducting Channels in Alkaline Polymer Electrolytes

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Alkaline polymer electrolytes (APEs) are an emerging material that enables the use of nonprecious-metal catalysts in electrochemical energy technology, such as fuel cell and water electrolysis.[1-2] Yet the OH^- conduction in APE has been of much lower efficiency than the H^+ conduction in its acidic counterpart (typically Nafion), leading to a large dissipative loss in energy conversion applications.

In the present work, we use coarse-grained molecular dynamics (CGMD) simulations to seek the optimal structure for APEs of high OH^- conducting efficiency.[3] We find that the most effective design for enhancing the hydrophobic/hydrophilic phase seperation microstructure in APE is to properly introduce a hydrophobic side chain onto the polymer backbone and to keep it away from the cationic functional group (Figure 1). This strategy is new and has not been well explored before.

Guided by the CGMD simulations, highly efficient OH^- conducting APEs (called *a*QAPS) have been realized experimentally. The OH^- conduction in *a*QAPS turns out to be as efficient as the H^+ conduction in Nafion (greater than 0.1 S/cm at 80ºC under moderate ion-exchange capacity of 1.0 mmol/g, Figure 2).

These findings have not only furthered our understanding about the ionic channels in APE, but also provided a general strategy for the rational design of polymer electrolytes. Detailed will be provided in the presentation.

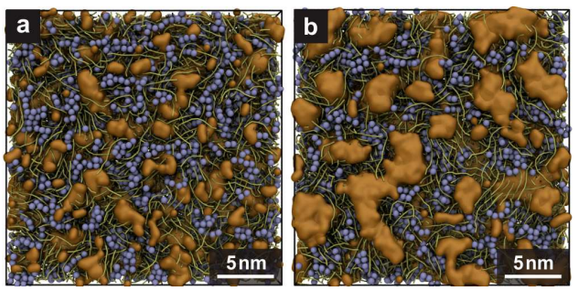

Figure 1. Coase-grained MD simulations on the phase seperation structure of APEs with a short (a) or long (b) hydrophobic side chain. Blue beads are hydrophilic species, yellow parts are the hydrophobic domain, and green ropes are polymer backbones.

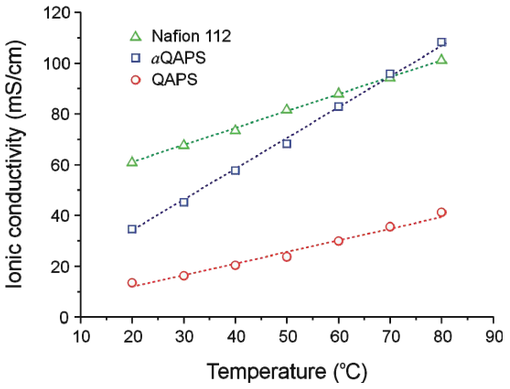

Figure 2. Ionic conductivity of *a*QAPS compared with Nafion 112 and conventional QAPS membranes.

References

1. Lu, S., Pan, J., Huang, A., Zhuang, L. & Lu, J. Alkaline polymer electrolyte fuel cells completely free from noble metal catalysts. *Proc. Natl. Acad. Sci. U.S.A.* **105**, 20611-20614 (2008).
2. Xiao, L. Zhang, S., Pan, J., Yang, C., He, M., Zhuang, L. & Lu, J. First Implementation of Alkaline Polymer Electrolyte Water Electrolysis Working Only with Pure Water. *Energy Environ. Sci.* **5**, 7869-7871 (2012).
3. Pan, J., Chen, C., Zhuang, L. & Lu, J. Designing advanced alkaline polymer electrolytes for fuel cell applications. *Acc. Chem. Res.* **45**, 473-481 (2012).