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Materials informatics approach on neutron scattering data for the development of anion exchange membranes used for next-generation energy devices

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We aim to apply "materials informatics"(MI) for the development of high-performance anion-exchange membranes (AEM), which may be applied to next generation energy devices, such as non-platinum fuel cell hybrid vehicles and all solid secondary batteries. Currently, there are two major obstacles to using MI for such systems: the unclear higher-order (hierarchical) structure/function relationship of AEM and the lack of a comprehensive structural database under various practical temperature/humidity conditions. We plan to use scattering and simulation methods, in particular the unique CV-SANS (Contrast-Variation Small Angle Neutron Scattering) technique with precise Partial Scattering Function (PSF) analysis, to obtain an accurate structure of each component in real AEMs under practical operating conditions and also to target various AEMs prepared by Radiation Graft Polymerization (RGP), which allows to impart new functionality to graft polymers while maintaining the mechanical and thermal properties of base polymers. A structural dataset will be defined through CV-SANS, microscopy and simulations, and we aim to create new optimized AEM through machine learning algorithms using this database. In our recent studies on hydrated proton exchange membrane (PEM) systems we introduce CV method to conventional SANS measurements to give multiple profiles for one sample under one operation condition (i.e. multiple equations), which are necessary for unique PSF analysis to determine precise structure of each component [1, 2]. Examples of PSF analysis of CV-SANS data collected at KWS-2 SANS instrument and the plans on using MI for next generation AEMs will be reported.

[1] Y. Zhao et al., Macromolecules 54, 4128 (2021).
[2] Y. Zhao et al., Macromolecules in press (2022).

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