Excessive molecular structure and properties determination of different types of alkyl sulfonated polyimide (ASPI) with universal neural network potential (UNNP)

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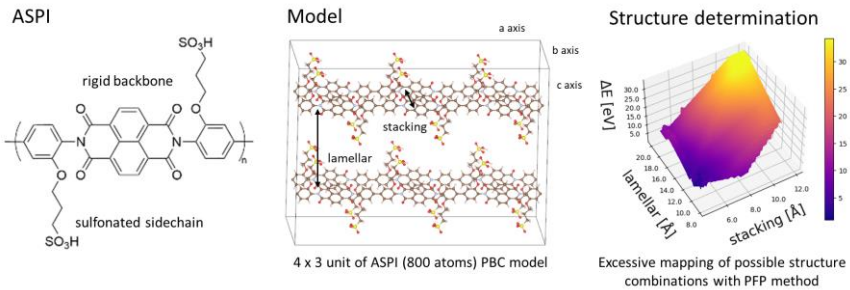
Alkyl sulfonated polyimide (ASPI) with rigid aromatic backbones and sulfonated alkyl side chains show promising proton conductivity especially with water uptake[1], and possible application as ion channels in Li-ion batteries. However, the role of backbone rigidity and side chain contribution for the lyotropic liquid crystal properties remains unclear.

Neural Network Potentials (NNP) are rapidly gaining attention due to the powerful combination of neural networks with large-scale datasets. Furthermore, the so-called Universal Neural Network Potentials (UNNP) have been developed, which enables to handle many combinations of different elements on the periodic table and supporting the material discovery, determination of unknown/new structures and extend the limitation of quantum mechanics.

The UNNP called as PreFerred Potential[2] (PFP) was used to determine the molecular structure of different types of ASPI with an excessive mapping of possible structure combinations. The characterization and elucidation of molecular properties and investigation of molecular level solvation of these different ASPI types can aid the understanding of lyotropic liquid crystal formation and the further design of ASPI types, and the usage of them as coating/ion channel material in Li-ion batteries.



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