

Study on ion transport in polyelectrolytes:
Molecular dynamics

이원보[†]
서울대학교
(wblee@snu.ac.kr[†])

In the current fuel cells and redox flow battery systems, the low ion conductivity and poor stability have been a main bottle neck for the commercialization of ion conducting electrolytes. For solving such highly challenging problems and understanding the fundamental mechanism between the conducting ion and matrix, the system will be investigated by molecular dynamics. In the presentation, preliminary studies on ion transport in polyelectrolytes will be discussed, including the prediction of microstructures, the effect of confinement on ion transport, and simulations details.