Theoretical investigation toward Li-ion conducting channel based on G-quadruplex

이경민, 이지은, 이상영[1], 곽상규†
울산과학기술원; [1]연세대학교
(skkwak@unist.ac.kr†)

Increasing demand for novel electrolytes is emerging as an important issue in the field of rechargeable batteries. Solid electrolytes are considered as rising candidates to replace liquid electrolytes since they have superior energy density and no safety concerns. However, the practical use of solid electrolytes is limited due to its low ionic conductivity and high interfacial resistance. In this study, we focused on G-quadruplex, a biogenic material with 1D ionic molecular tubes which consist of π-π stacked quartets, as a potential Li^+ conducting substance. First, thermodynamically favorable stacking sequence of G-quadruplex were determined through molecular mechanics simulations. Second, a competitive Li^+ migration energy barrier was calculated (c.a. ~20 kJ/mol), which is comparable to the reported superionic conductors. Third, structural stability of G-quadruplex in solid state and trapped anion position were elucidated via molecular dynamics simulations. Finally, unidirectional and single-ion conducting behavior of G-quadruplex was examined by applying electric field. In conclusion, we propose G-quadruplex as a promising material for solid electrolyte application.