Theoretical Investigation of G-quadruplex based Novel Single-Ion Conductor

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Electrolytes play key roles in rechargeable batteries. Liquid electrolytes have high ionic conductivity but suffer from performance degradation and safety problems. Solid electrolytes, especially single-ion conductors cause little of such problems, but low ionic conductivity limits their applications. Thus, the development of novel electrolyte, which has advantages of both electrolytes, is an important task. To achieve high ionic conductivity and cation transference number, we adopted G-quadruplex structure, 1D molecular tube made from π-π stacking of stable quartets, which enables rapid cation transport. Through series of molecular mechanics (MM) simulations, building block candidates that are suitable for single-ion conductors were investigated. First, quartet formation energy was calculated to predict the stability of quartet structure. Second, stacking energy was estimated to evaluate the formability of molecular tubes. Finally, Li ion migration energy barrier was compared with other solid electrolytes. The candidates that can form molecular tubes turned out to have ion migration barrier about ~20 kJ/mol, which is competitive compared to reported super-ionic conductors.