The Exterior of Single-Walled Carbon Nanotubes as a Millimeter-Long Cation-Preferring Nanochannel: Contribution of Cation-π Interaction

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Cation-π interaction, a noncovalent interaction between adjacent cations and a π-plane, has a crucial role in nature or artificial system. Especially, various cation-preferential transport phenomenas that occur in π-system have been widely reported. However, the cation-π interaction as a transport mechanism along a π-system has not been confirmed due to the challenges to verify preferential transport experimentally. In this study, preferential transport phenomena on the surface of single walled carbon nanotubes (SWNT) was successfully shown by the formation of dark line (positively charged) and bright lines (negatively charged) along the nanotubes in scanning electron microscopy. Furthermore, the mechanism for migration behavior of solvated Na^+ and Cl^- ions around the wall of SWNT was investigated via molecular dynamics (MD) simulations. In MD simulations, the cation-preferring transport results in the formation of positively charged salt crystals along the SWNT (with a cation-to-anion ratio of 0.53:0.47) followed by anion counter-migration. Our result showed that the cation-π interaction was responsible for the cation preference during ionic transport along the SWNT.