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The Effect of Carbon Nanotube Diameter on Hydration of Critical Material Ions from E-waste

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Critical materials such as lithium, nickel, and cobalt play an important role in the sustainable development of society. However, establishing a reliable supply of these critical materials has been a challenge for the USA. Meanwhile, electronic waste (E-waste) has become a societal burden due to the quick spread of electronic devices and electric cars. E-waste contains a large amount of exposed lithium, nickel, and cobalt, which will pollute the soil and water if not disposed of properly. Thus, highly efficient technology that can recover critical materials from E-waste can help reduce the detrimental effects of E-waste on the environment and resolve the supply chain issue for those critical materials. One challenge of recovering critical materials from E-waste is developing a separation technology that can differentiate between the materials themselves. Nanoporous materials have shown their exceptional potential in separating substrates with similar chemical and physical features. However, the creation of such nanoporous materials must be based on a full understanding of the molecular thermodynamics of ionic hydration within nanoscale confinement. This work investigates the hydration structure and dynamics of three critical material ions for lithium-ion batteries (Li^{2+}, Ni^{2+}, and Co^{2+}) within carbon nanotubes with a diameter from 1.0-2.0 nm using molecular simulations. We deploy classical and ab initio molecular dynamics (MD) simulations to investigate the structural and dynamic properties of water molecules with those ions within the carbon nanotubes. We also explore the development of deep learning force fields that enable us to investigate the ionic hydration within carbon nanotubes as accurately as ab initio MD simulations, but much faster. The simulation-revealed deviation will be used to develop membrane-based separation technology for recovering critical materials.

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