# Antioxidative Lithium Reservoir Based on Interstitial Channels of Carbon Nanotube Bundles

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Lithium (Li) metal has been considered as a potent candidate for next-generation battery anode. However, for commercial use, it is urgent to solve the safety problem caused by electrochemical instability. Here, we suggest a new concept of antioxidative Li reservoir based on interstitial channels of single-walled carbon nanotube (SWCNT) bundles via theoretical approach. Using molecular dynamics (MD) simulations considering the cation-pi interaction, we observed that the Li in the bundle's interstitial site is thermodynamically stable even when the SWCNT bundle is exposed to an oxidative environment such as water. Through the combined methodology of MD and density functional theory (DFT), we demonstrated that Li confined at the interstitial site is more stable than Li adsorbed at the bundle surface or groove site. Based on the simulation results, we also proposed the lithiation/delithiation mechanism of SWCNT bundles in electrolyte environment. Taking advantage from the confinement effect of the interstitial channels, the SWCNT bundles has great potential as a Li reservoir to withstand the oxidative environment.