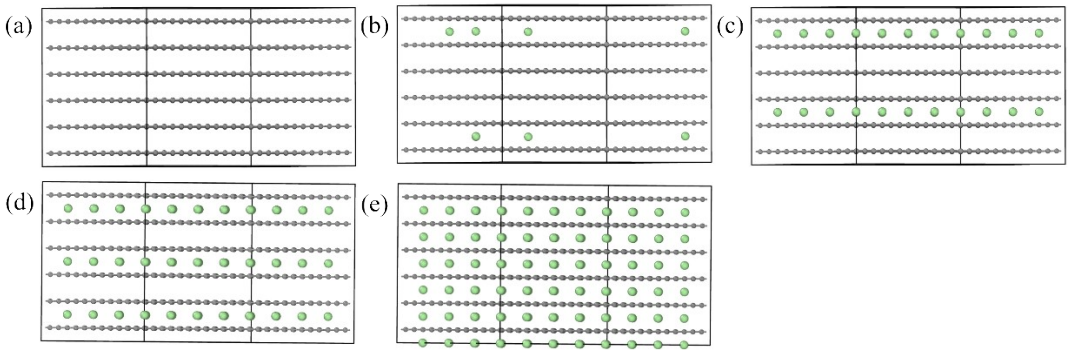

Figure S1 (a)，(b)，(c)，(d)and (e) are respectively the simulated initial models of Li_xC_6 (X=0.02-1).

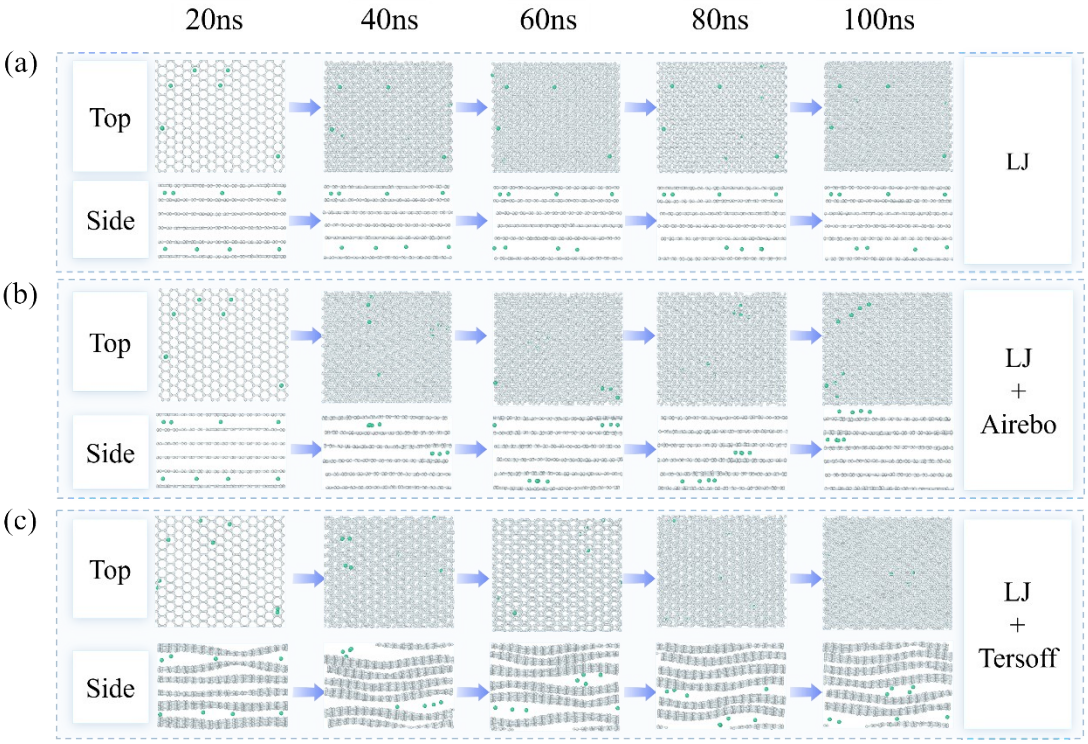

Figure S2 MD simulations of the top and side views of the $Li_{0.02}C_6$ model were carried out within 100ns. During the simulations, (a) the LJ potential function, (b) the Airebo potential function and (c) the Tersoff potential function describe the interaction of C-C bonds between graphite layers. where grey represents carbon atoms and green represents lithium atoms.

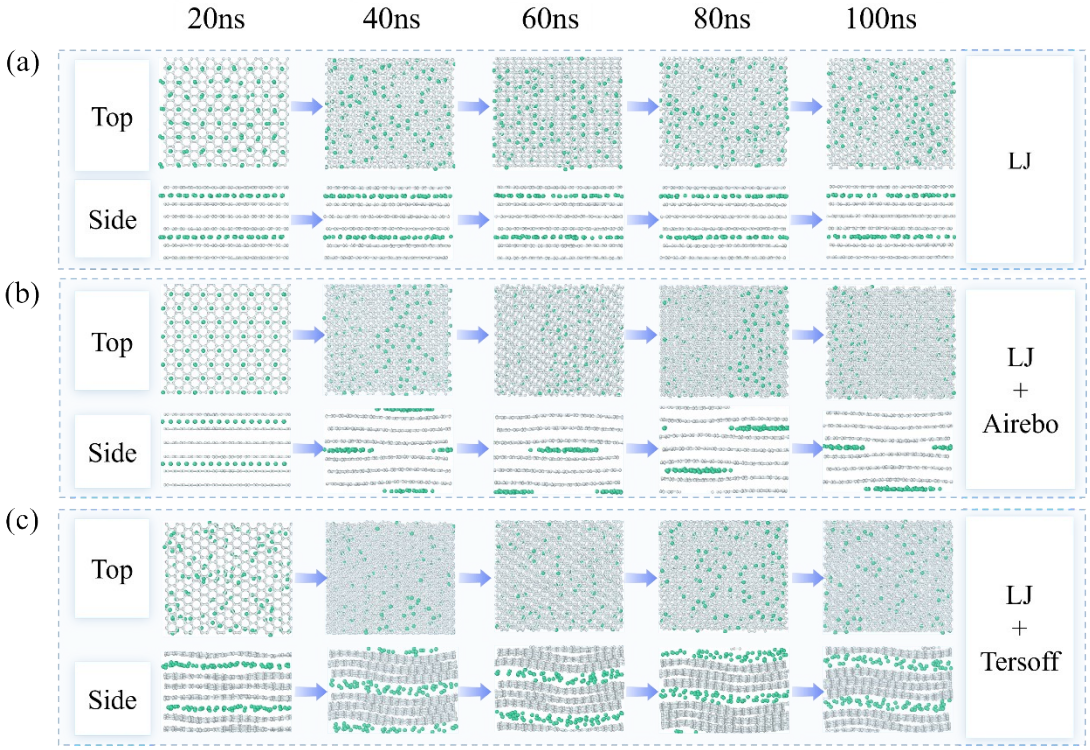

Figure S3 MD simulations of the top and side views of the $Li_{0.33}C_6$ model were carried out within 100ns. During the simulations, (a) the LJ potential function, (b) the Airebo potential function and (c) the Tersoff potential function describe the interaction of C-C bonds between graphite layers. where grey represents carbon atoms and green represents lithium atoms.

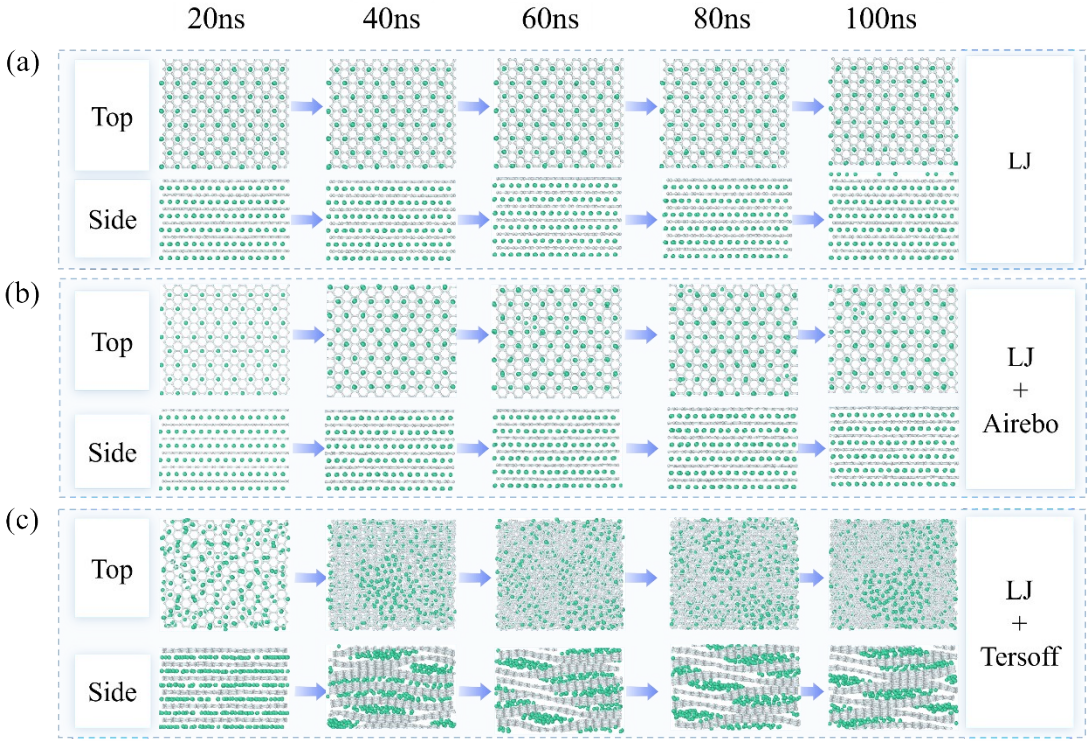

Figure S4 MD simulations of the top and side views of the $Li_{0.5}C_6$ model were carried out within 100ns. During the simulations, (a) the LJ potential function, (b) the Airebo potential function and (c) the Tersoff potential function

describe the interaction of C-C bonds between graphite layers. where grey represents carbon atoms and green represents lithium atoms.

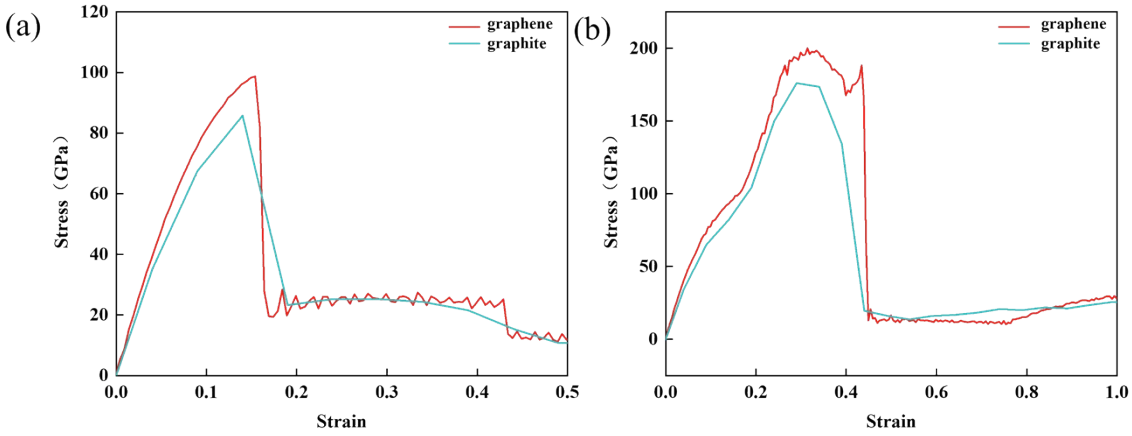

Figure S5 The stress-strain curves of graphene with different layers: (a) Represents the stress-strain curves of monolayer graphene and six-layer graphite obtained using the AIREBO potential function. (b) Represents the stress-strain curves of monolayer graphene and six-layer graphite obtained using the Tersoff potential function.

Table S1

Diffusion Coefficients of Lithium ions (cm^2 /sec)				
	This Work		MC[1]	DFT[2]
	Airebo	Tersoff		
$Li_{0.02}C_6$	1.3955×10^{-6}	4.95167×10^{-6}	/	/
$Li_{0.2}C_6$	/	/	1.43×10^{-8}	7.04×10^{-6}
$Li_{0.33}C_6$	6.66×10^{-7}	3.63833×10^{-6}	1.40×10^{-8}~	6.71×10^{-6}
$Li_{0.5}C_6$	3.26075×10^{-8}	3.22202×10^{-6}	7.74×10^{-12}~7.59×10^{-9}	6.66×10^{-6}
LiC_6	3.98×10^{-9}	8.53×10^{-7}	7.70×10^{-10}	6.83×10^{-6}

[1] Persson K, Sethuraman V A, Hardwick L J, et al. Lithium diffusion in graphitic carbon[J]. The journal of physical chemistry letters, 2010, 1(8): 1176-1180.

[2] Kresse, G. Furthmuller, Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a PlaneWave Basis Set. J. Comput. Mater. Sci. 1996, 6, 15–50.