Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Enhancing the efficiency of lithium intercalation in carbon nanotube bundle using surface functional groups

supplementary Information

Shiyan Xiao,[†] Hong Zhu,[†] Lei Wang,[†] Liping Chen,[†] and Haojun Liang*,[‡,¶]

CAS Key Laboratory of Soft Matter Chemistry, Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China., CAS Key Laboratory of Soft Matter Chemistry, Collaborative Innovation Center of Chemistry for Energy Materials, Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China., and Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, P. R. China.

E-mail: hjliang@ustc.edu.cn

Phone: +86 (0)551 63607824. Fax: +86 (0)551 63607824

*To whom correspondence should be addressed

[†] CAS Key Laboratory of Soft Matter Chemistry

[‡] CAS Key Laboratory of Soft Matter Chemistry, Collaborative Innovation Center of Chemistry for Energy Materials

[¶]Hefei National Laboratory for Physical Sciences at Microscale

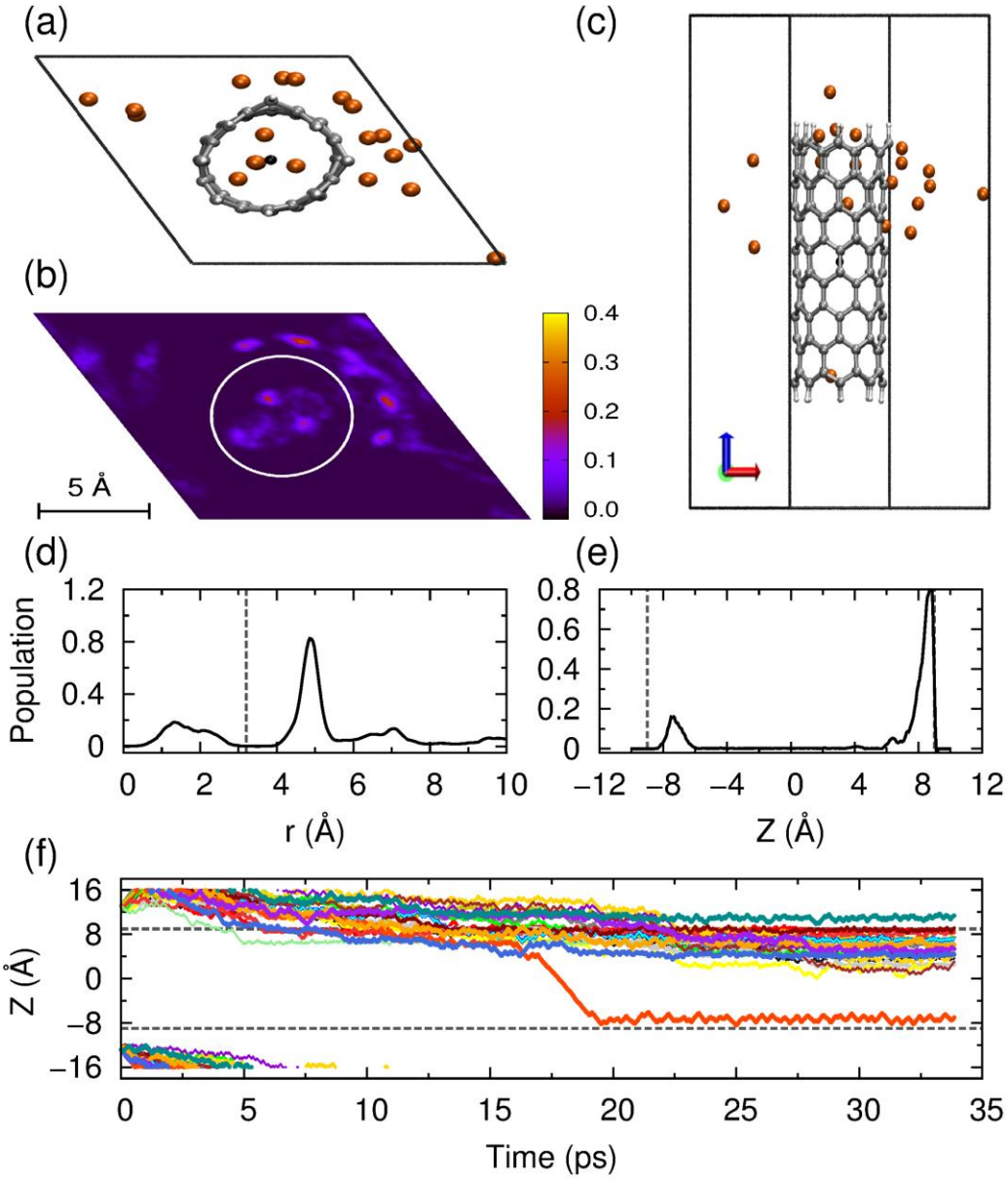

Figure S1 Behavior of the twenty lithium ions intercalating and diffusing inside or between CNTs. The system was simulated in a hexagonal box with dimensions 15.0×15.0×32.0 $Å^3$. (a) Typical snapshot of the unit cell, view from the top. (b) Distribution of the lithium ions in the x-y plane. (c) Typical snapshot of the unit box, side view. (d) Radial distribution of the lithium ions, and the vertical dashed line represents the wall of nanotube. (e) Axial distribution of the ions within CNT, only calculated for the ions within the nanotube. The two ends of CNT are indicated by the two vertical dashed lines. (f) The z-position as a function of simulation time (ps) for each lithium ion. The upper and lower dashed gray horizontal lines denote the top and bottom ends of CNT, respectively. Because the simulation is performed under periodic boundary condition, these ions that move down towards the bottom edge of the simulation box will simultaneously appear at the top edge of the box.

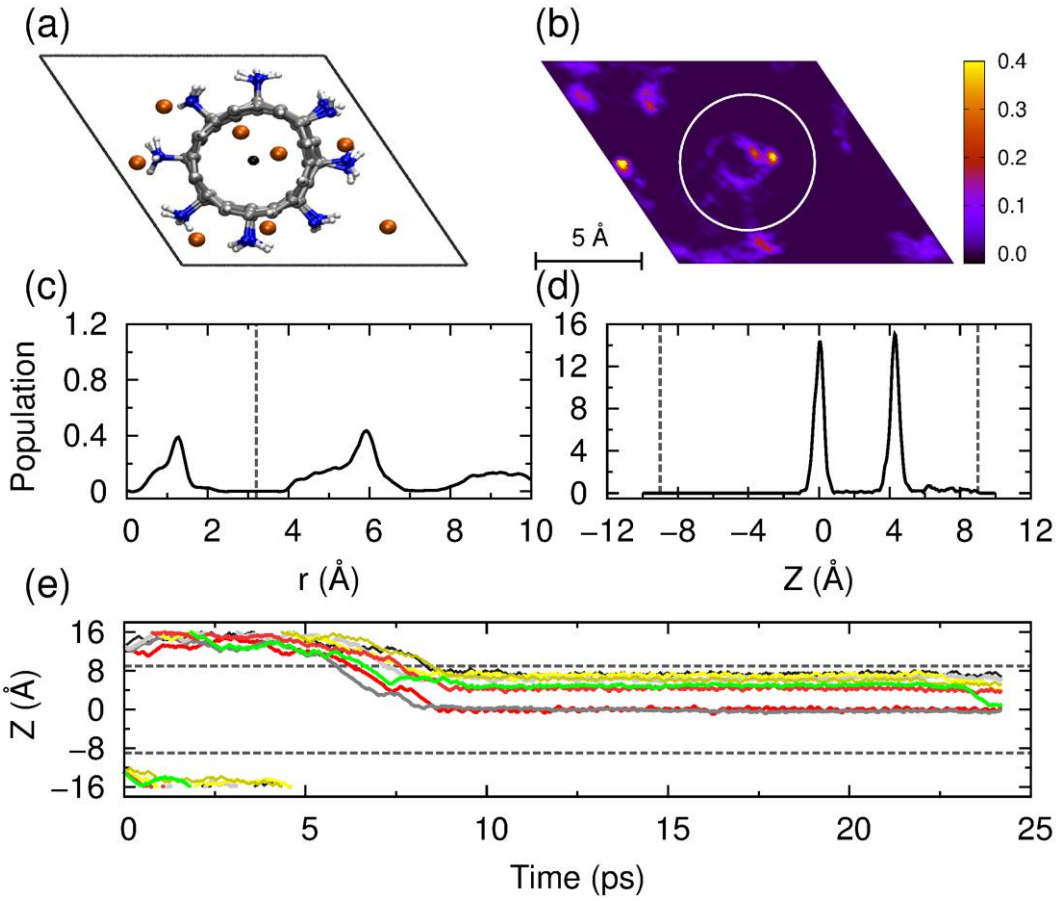

Figure S2 Behavior of the eight lithium ions intercalating and diffusing inside or between CNTs. The system was simulated in a hexagonal box with dimensions 13.0×13.0×32.0 $Å^3$. (a) Typical snapshot of the unit cell, view from the top. (b) Distribution of the lithium ions in the x-y plane. (c) Radial distribution of the lithium ions, and the vertical dashed line represents the wall of nanotube. (d) Axial distribution of the ions within CNT, only calculated for the ions within the nanotube. The two ends of CNT are indicated by the two vertical dashed lines. (e) The z-position as a function of simulation time (ps) for each lithium ion. The upper and lower dashed gray horizontal lines denote the top and bottom ends of CNT, respectively. Because the simulation is performed under periodic boundary condition, these ions that move down towards the bottom edge of the simulation box will simultaneously appear at the top edge of the box.

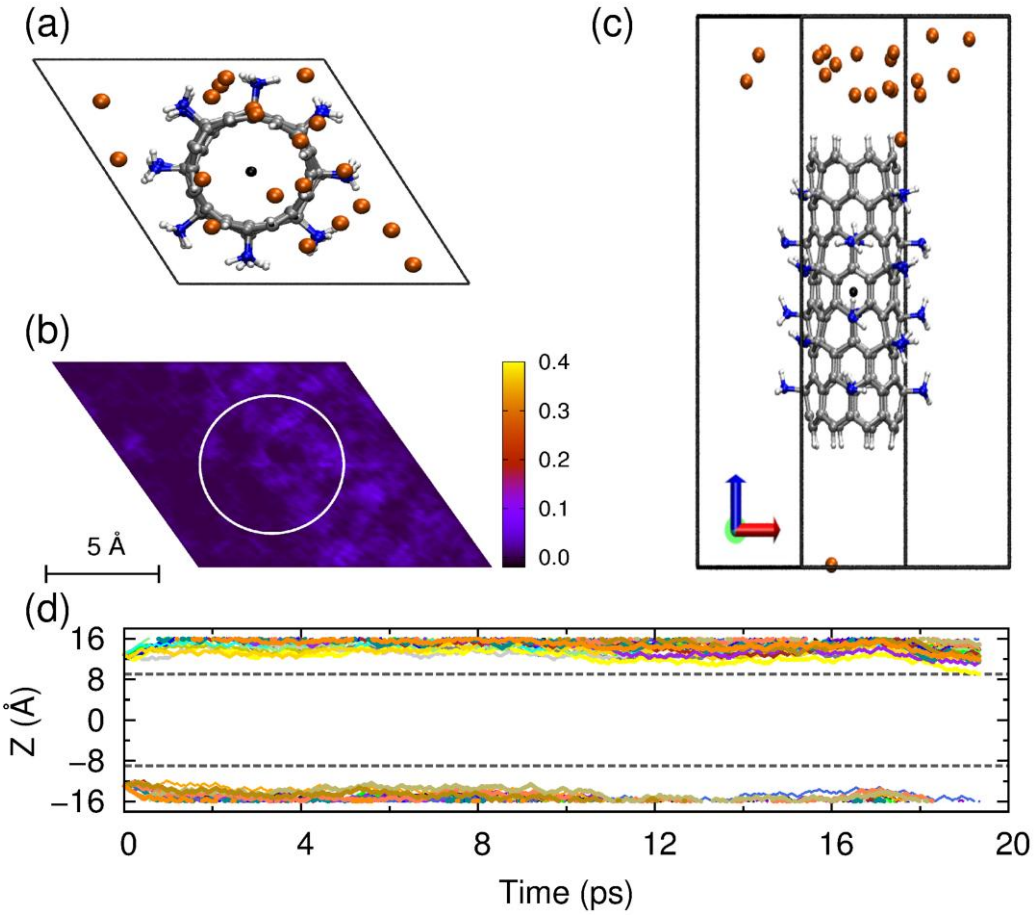

Figure S3 Behavior of the twenty lithium ions intercalating and diffusing inside or between $–NH_2$ functionalized CNTs. The system was simulated in a hexagonal box with dimensions 13.0×13.0×32.0 $Å^3$. (a) Typical snapshot of the unit cell, view from the top. (b) Distribution of the lithium ions in the x-y plane. (c) Typical snapshot of the unit box, side view. (d) The z-position as a function of simulation time (ps) for each lithium ion. The upper and lower dashed gray horizontal lines denote the top and bottom ends of CNT, respectively. Because the simulation is performed under periodic boundary condition, these ions that move down towards the bottom edge of the simulation box will simultaneously appear at the top edge of the box.