

## Supporting Information

# Ionic Liquids Filled Single-Walled Carbon Nanotubes for Flow-Induced Energy Harvesting

Yongji Guan,<sup>†</sup> Wenqiong Chen,<sup>†</sup> Jiao Zhang,<sup>†</sup> Fulong Yang,<sup>†</sup> Chao Du,<sup>†</sup> Xiaoping Zhang,<sup>\*,†</sup>

Youquan Deng<sup>\*,‡</sup>

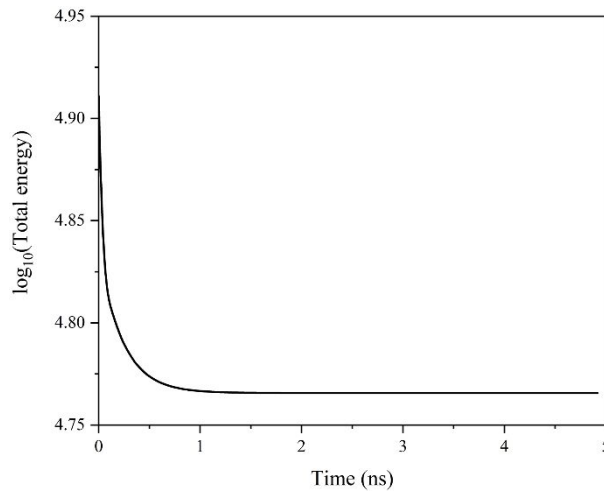
<sup>†</sup>Institute of Optoelectronics and Electromagnetic Information, School of Information Science and Engineering, Lanzhou University, Lanzhou, 730000, People's Republic of China.

<sup>‡</sup>Centre for Green Chemistry and Catalysis, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou, 730000, People's Republic of China.

\*Corresponding author. Prof. Xiaoping Zhang, E-mail: [zxp@lzu.edu.cn](mailto:zxp@lzu.edu.cn).

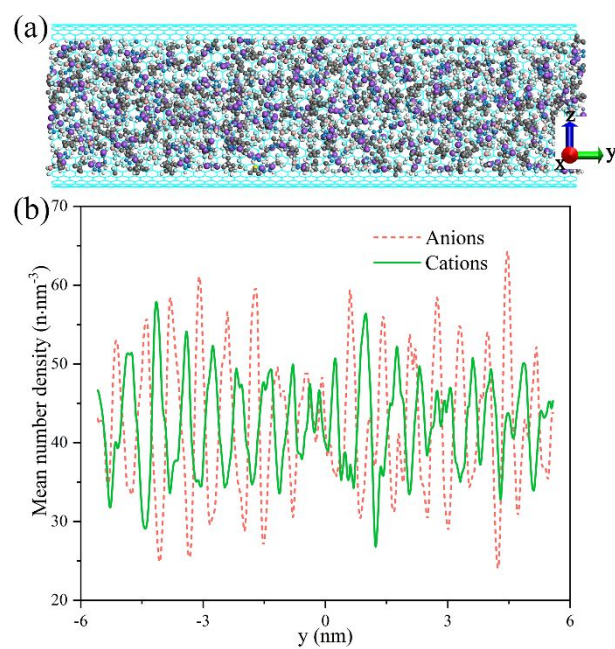
\*Corresponding author. Prof. Youquan Deng, E-mail: [ydeng@licp.cas.cn](mailto:ydeng@licp.cas.cn).

Figure S1 presents the variation of total energy of the simulation system consists of [Emim][BF<sub>4</sub>] and graphene nano-channel with relaxation time steps. From Figure S1, we can find the total energy of the simulation gradually decreases with the increasing of the simulation times then converges to a constant. So the simulation system can be regarded as reaching the equilibration.

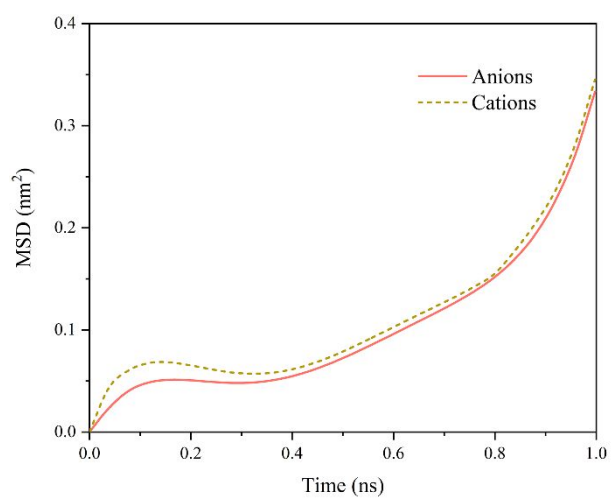


**Figure S1.** The variation of total energy of the simulation system consists of [Emim][BF<sub>4</sub>] and SWCNT with relaxation time steps.

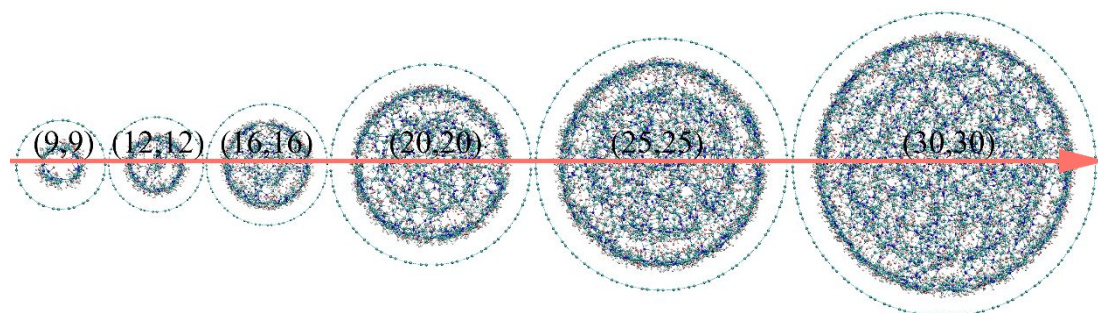
After the system reached the equilibration, to observe the spatial distribution of ions in axial direction, we calculate the mean number density of ILs, cations and anions, plotted in Figure S2. Clearly, the mean number of ILs fluctuates across a fixed value and no distinct layers occur along axial direction. It is not taking the ions distribution of ILs in axial direction into consideration when calculating the flow induced voltage.



**Figure S2.** (a) The axial equilibrium structure of the ILs [Emim][BF<sub>4</sub>] inside a (25,25) SWCNT, (b) the mean number density of cations and anions in axial direction at T = 300 K.

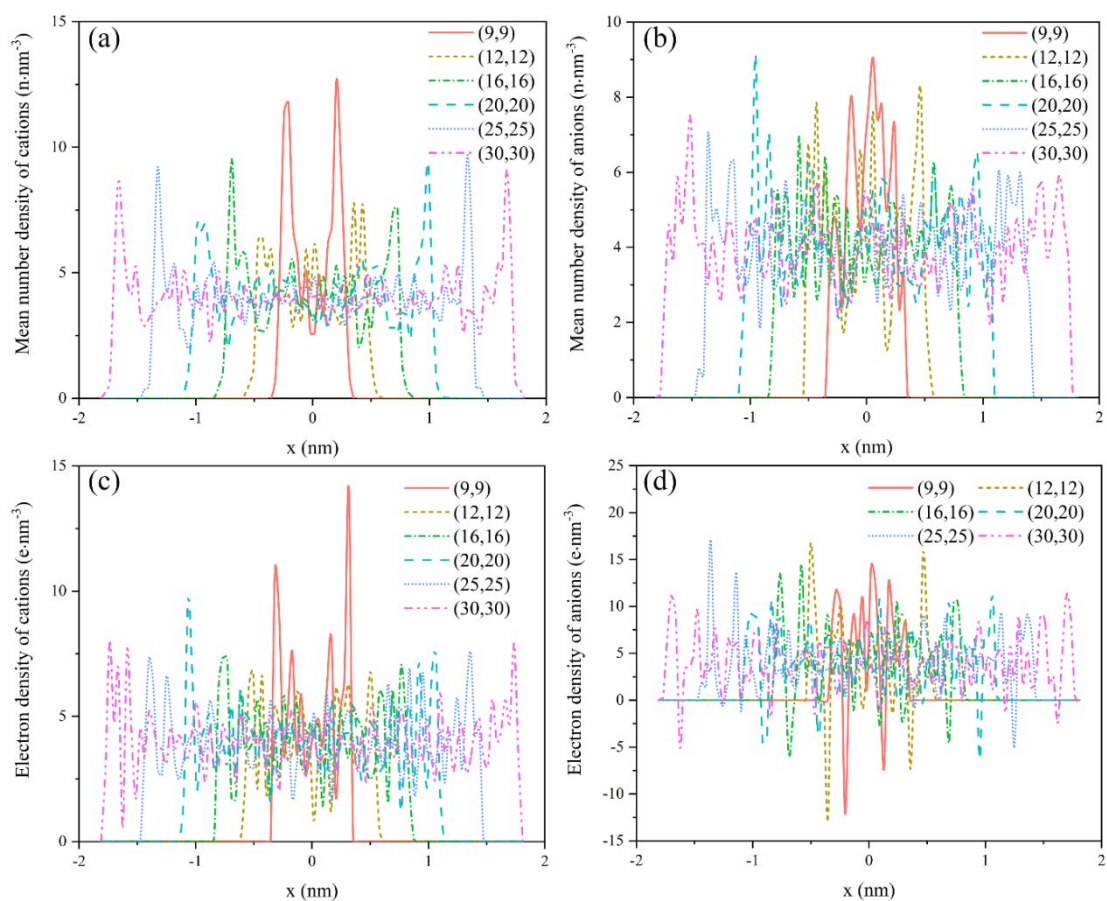


**Figure S3.** MSDs of cations and anions for ILs [Emim][BF<sub>4</sub>] inside a (25,25) SWCNT at T = 300 K.

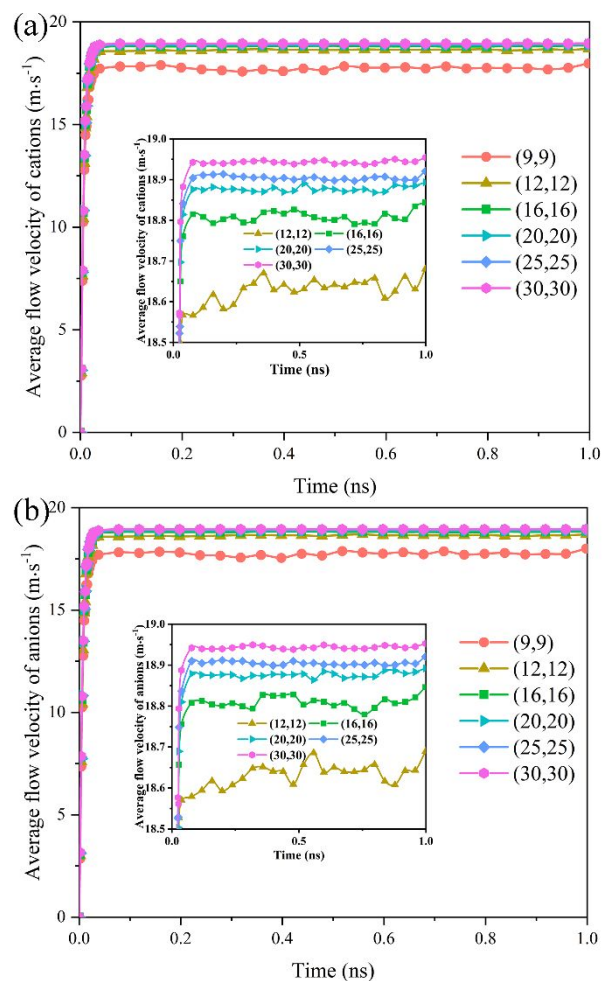


**Figure S4.** The equilibrated structures of ILs [Emim][BF<sub>4</sub>] inside SWCNT of different diameters at T = 300 K.

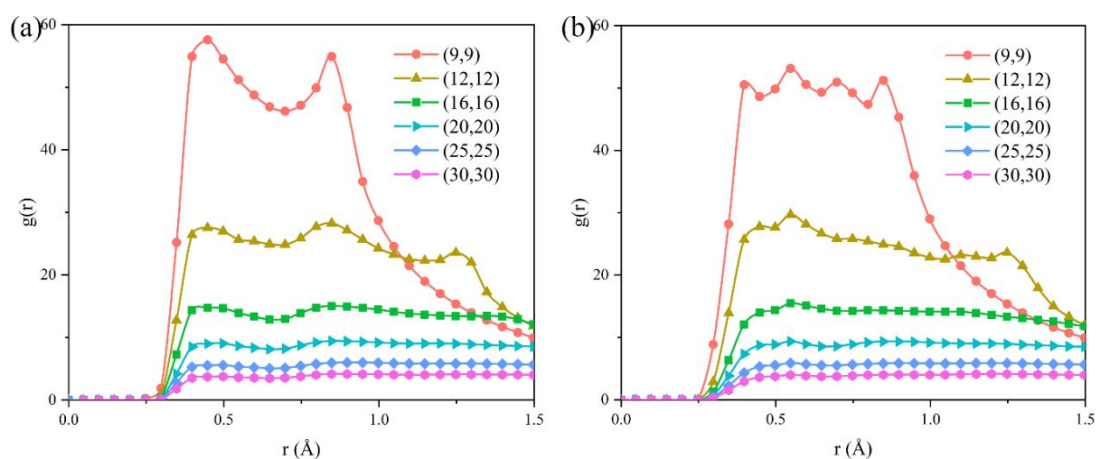
As showed in Figure S5a, b, although the peak value of anions is small than the peak value of cations near the wall of SWCNTs, the profile of the anions number density near the wall of SWCNTs has two separated peaks and is much broader compared to that of the cations. Thus anions and cations are maintained at basically the same number in the first solvation shell to satisfy the condition of charge neutrality. Additionally, anions are farther away from the wall of SWCNTs than cations.



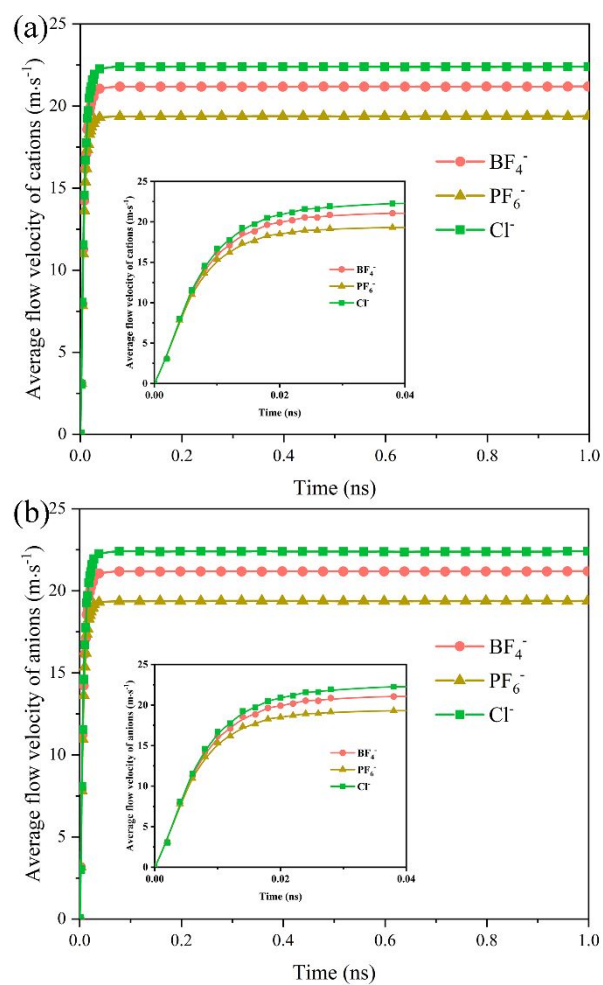
**Figure S5.** The radial number density of cations and anions inside SWCNT of different sizes in (a) and (b), the radial charge density of anions and cations inside SWCNT of different sizes in (c) and (d).



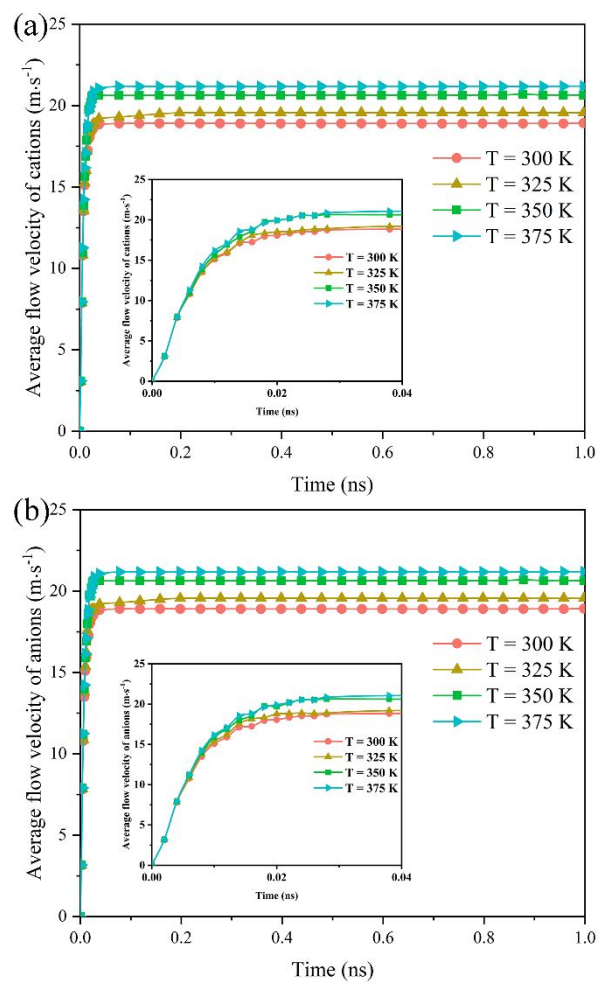
**Figure S6.** Average flow velocity of cations  $\text{Emim}^+$  in (a) and anions  $\text{BF}_4^-$  in (b), varying with time under different pore size at  $T = 300$  K.



**Figure S7.** Centre of mass RDFs for (a) cations and (b) anions around the carbon atoms of SWCNTs.

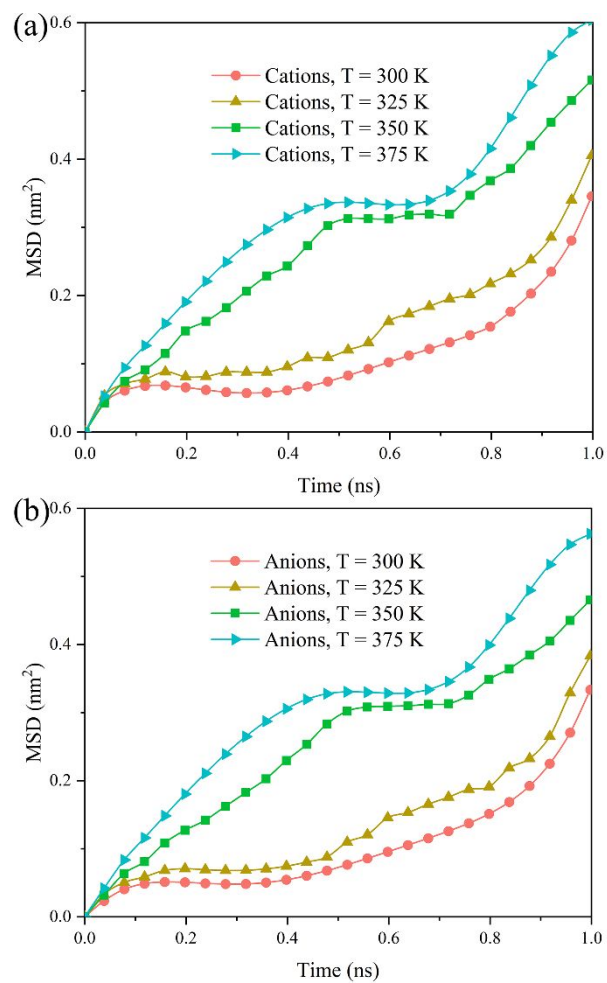


**Figure S8.** Average flow velocity of cations in (a) and anions in (b) for three kinds of ILs inside a (25,25) SWCNT at T = 375 K.



**Figure S9.** Average flow velocity of cations in (a) and anions in (b) for ILs [Emim][BF<sub>4</sub>] inside a (25,25) SWCNT at T = 300, 325, 350 and 375 K.





**Figure S10.** MSDs of cations in (a) and anions in (b) for ILs [Emim][BF<sub>4</sub>] inside (25,25) SWCNT at T = 300, 325, 350 and 375 K.