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Flow-Induced Voltage Generation by Driving Ionic Liquids over a Graphene Nano-Channel

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Introduction

Ionic Liquids (ILs)

- Soft functional materials
- Excellent physical and chemical properties
- Task-specific application

Nanostructure

- Complex technical processes
- Expensive experimental equipment
- Molecular dynamics (MD) simulation

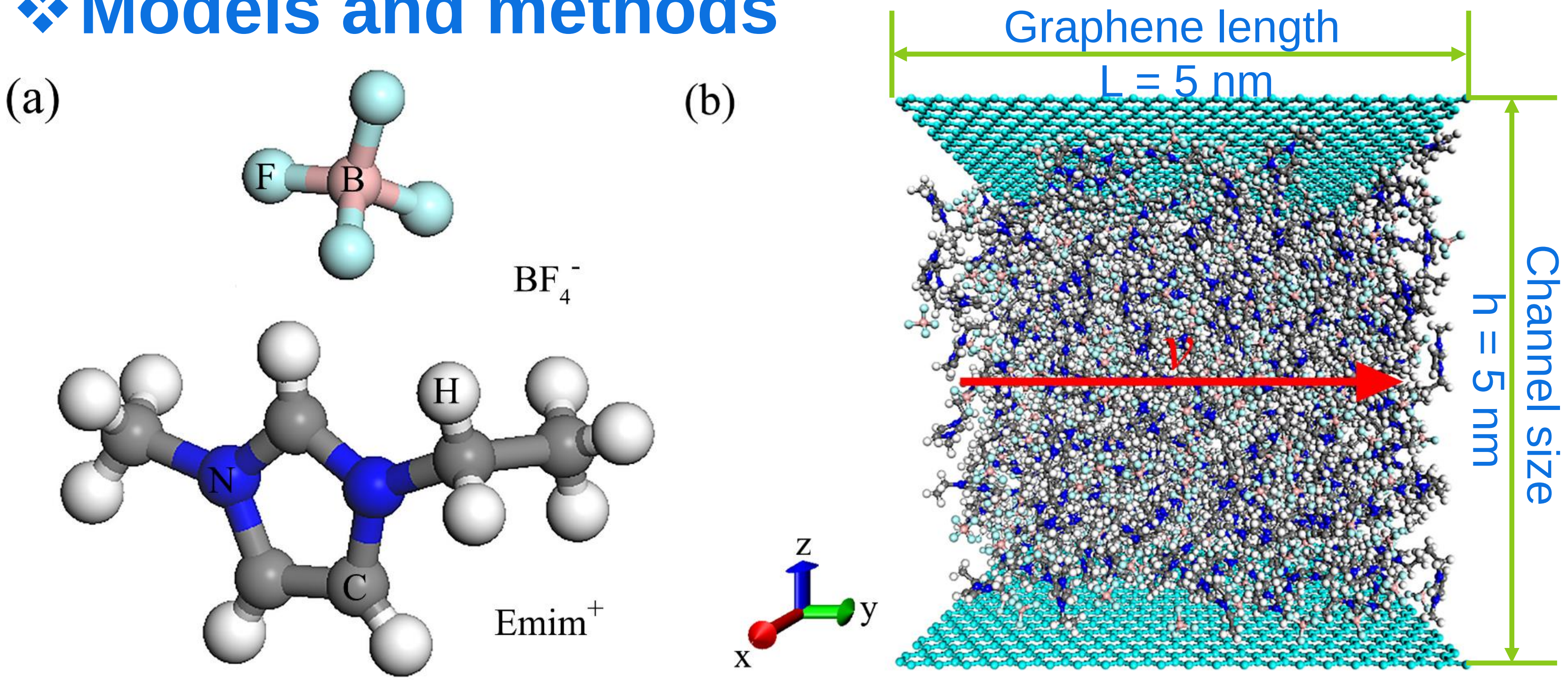
Energy Harvesting

- Powering the nano-electromechanical systems (NEMSs)
- Bio-molecular sensing
- Biomedical fields

1. Zhang, S.; Zhang, J.; Zhang, Y.; Deng, Y., Nanoconfined Ionic Liquids. Chem. Rev. 2017, 117, 6755-6833
2. Wang, Z. L., Self-Powered Nanosensors and Nanosystems. Adv. Mater. 2012, 24, 280-285.

Models and Methods

❖Models and methods



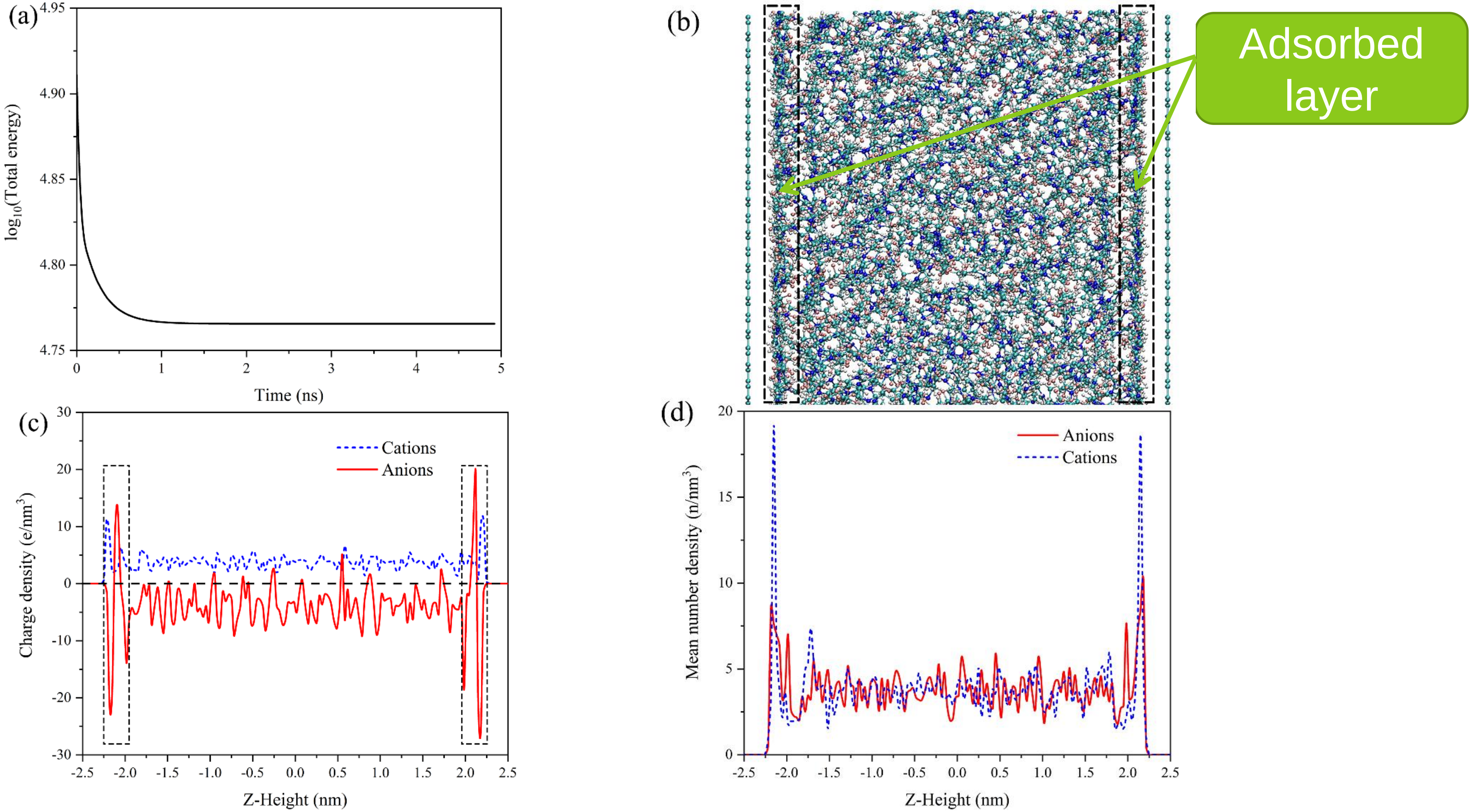
ILs + Graphene channel

MD simulation (20 ns, 300 K)

Acceleration: 0.001~0.2 nm ps^{-2}

Models and Methods

❖Charge and number density distribution



Models and Methods

❖ Calculated equation

Characteristic of Coulomb's law

Charge density distribution of Cations and anions

$$V = R\sigma eL\left(v^{+} - \frac{\left| \int_a^b \frac{1}{z^2}\rho^{-}(z)\,dz \right|}{\left| \int_a^b \frac{1}{z^2}\rho^{+}(z)\,dz \right|} v^{-} \right)$$

Combined effect of Cations and anions on free charge carriers

Range of Coulomb interaction

R : graphene sheet resistance e: electronic charge

σ : average free charge carrier density of graphene

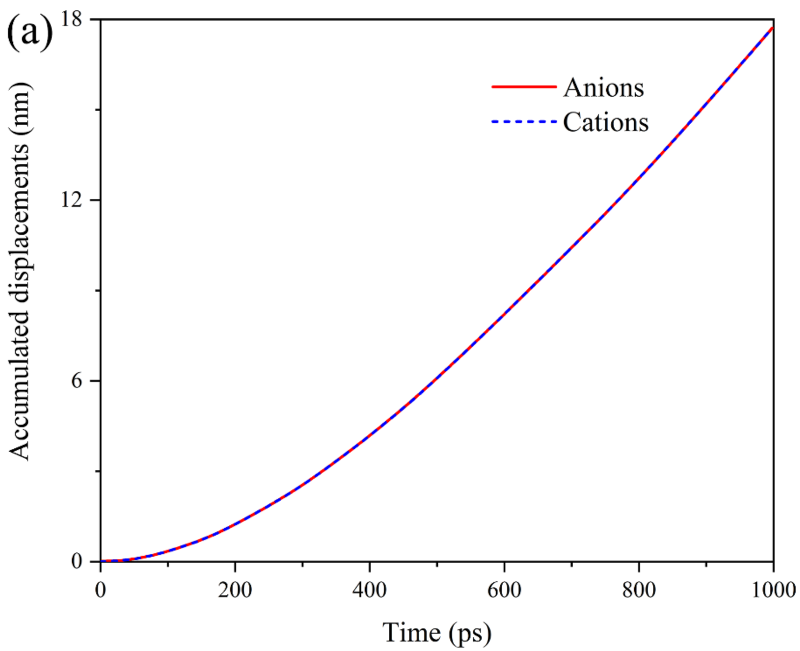
L : contact length of the ILs with graphene sheet

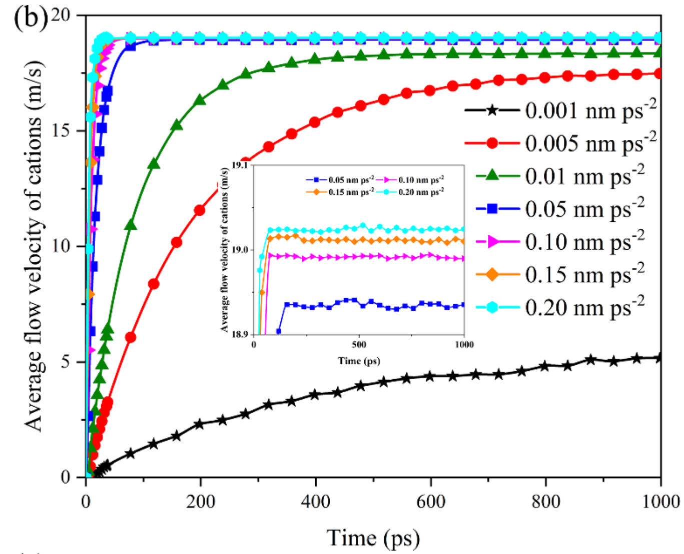
v^{+}, v^{-} : average flowing velocities of cations and anions

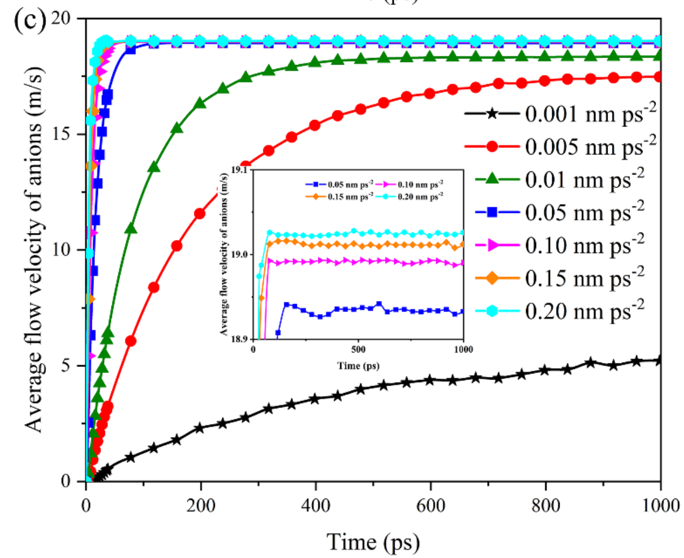
ρ^{+}, ρ^{+}: charge densities of cations and anions in Z direction

Results and Discussion

❖ Average flow velocity



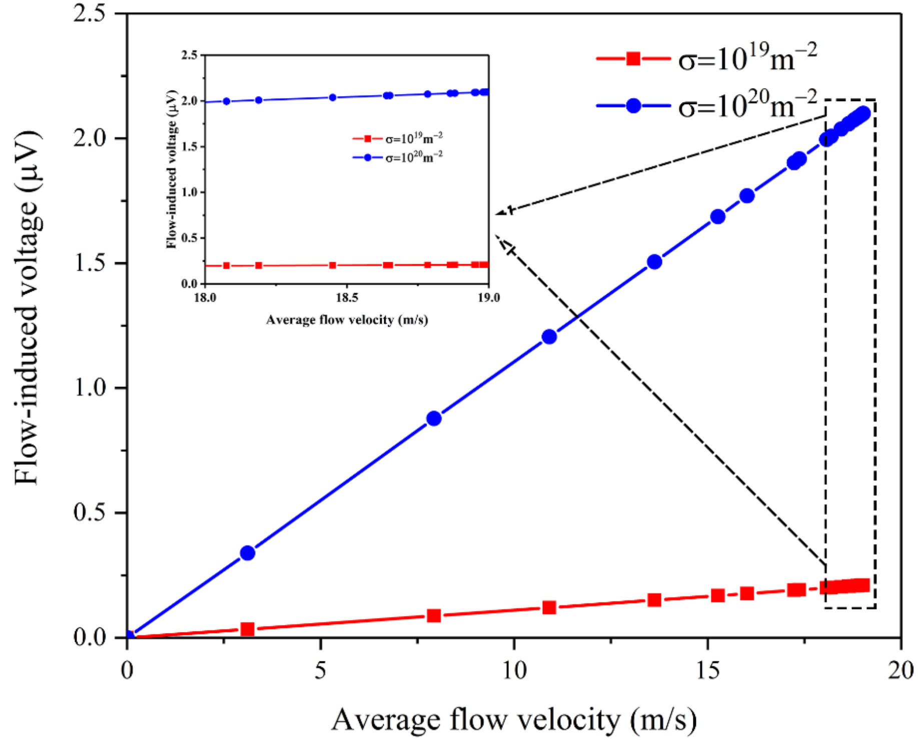




The average flow velocities of anions and cations nonlinearly increase to saturation.

Results and Discussion

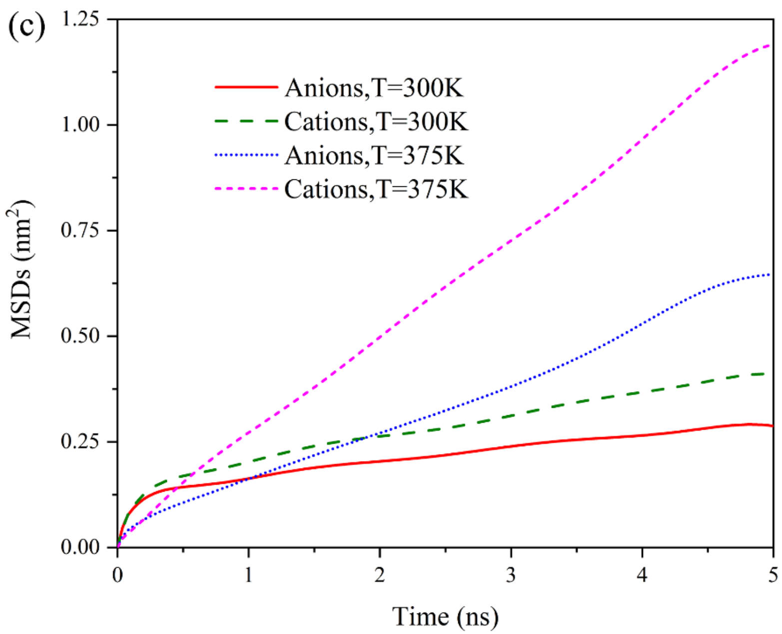
❖ Flow-induced voltage

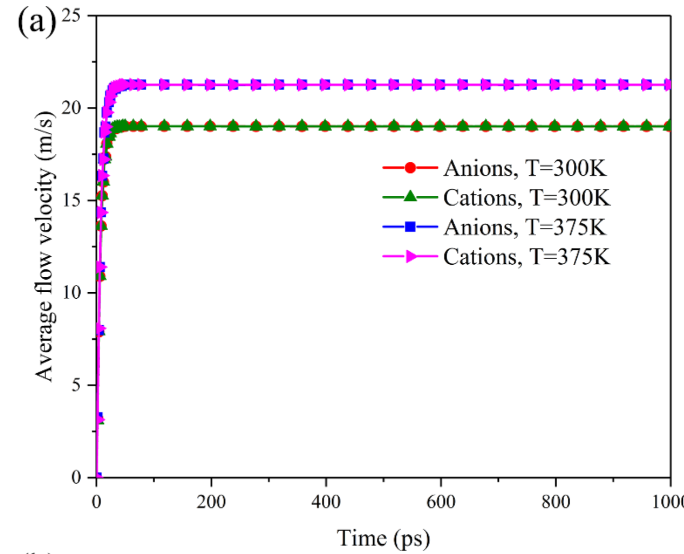


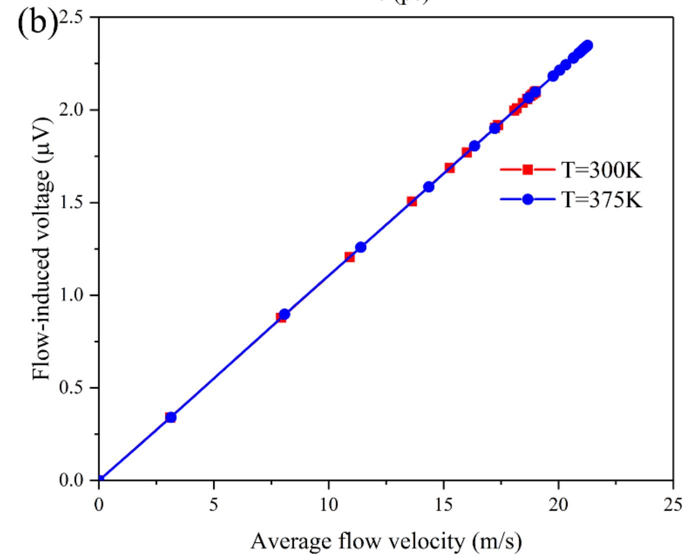
The flow-induced voltages is about 2.1 μV and tends to saturation as average flow velocity increases.

Results and Discussion

❖ Temperature effect



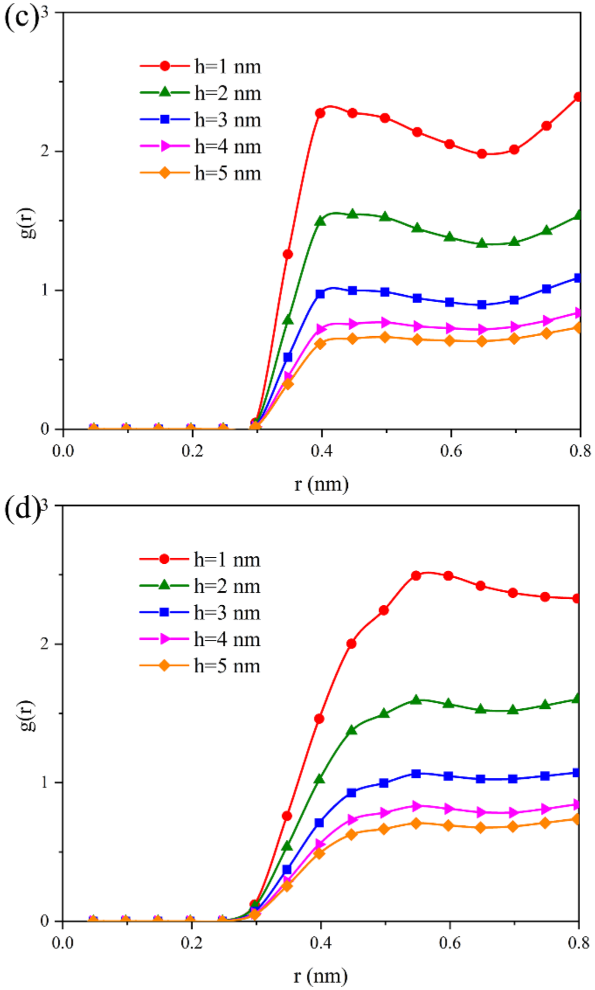




The flow-induced voltage (2.4 μV) has a significant increase at T = 375 K.

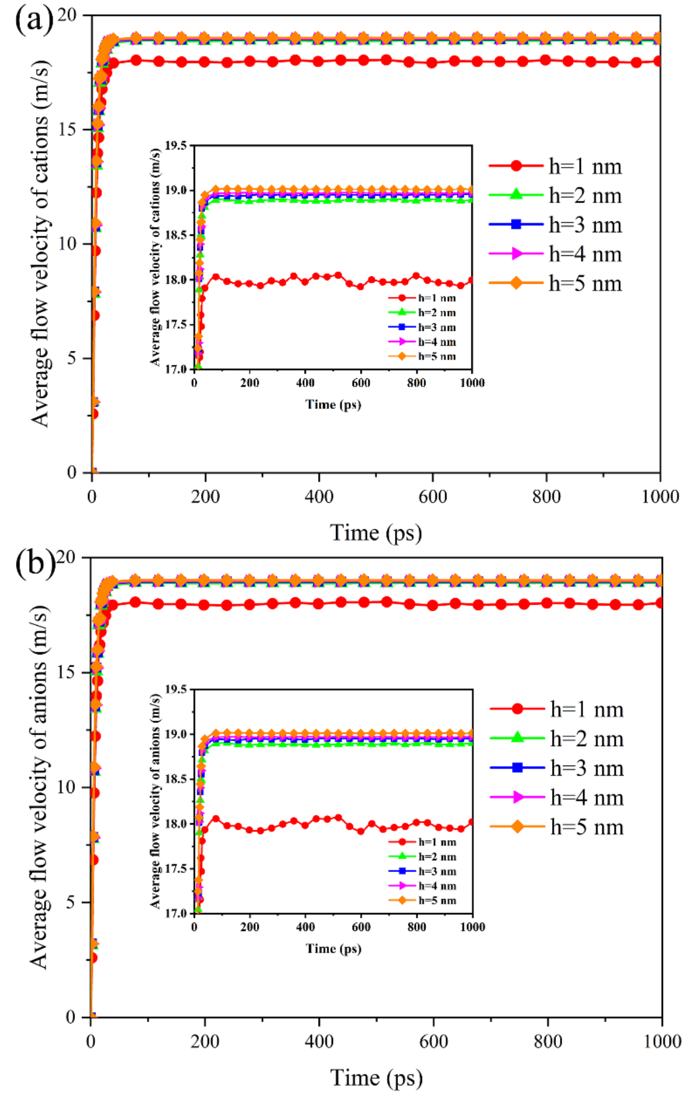
Results and Discussion

❖Channel size effect



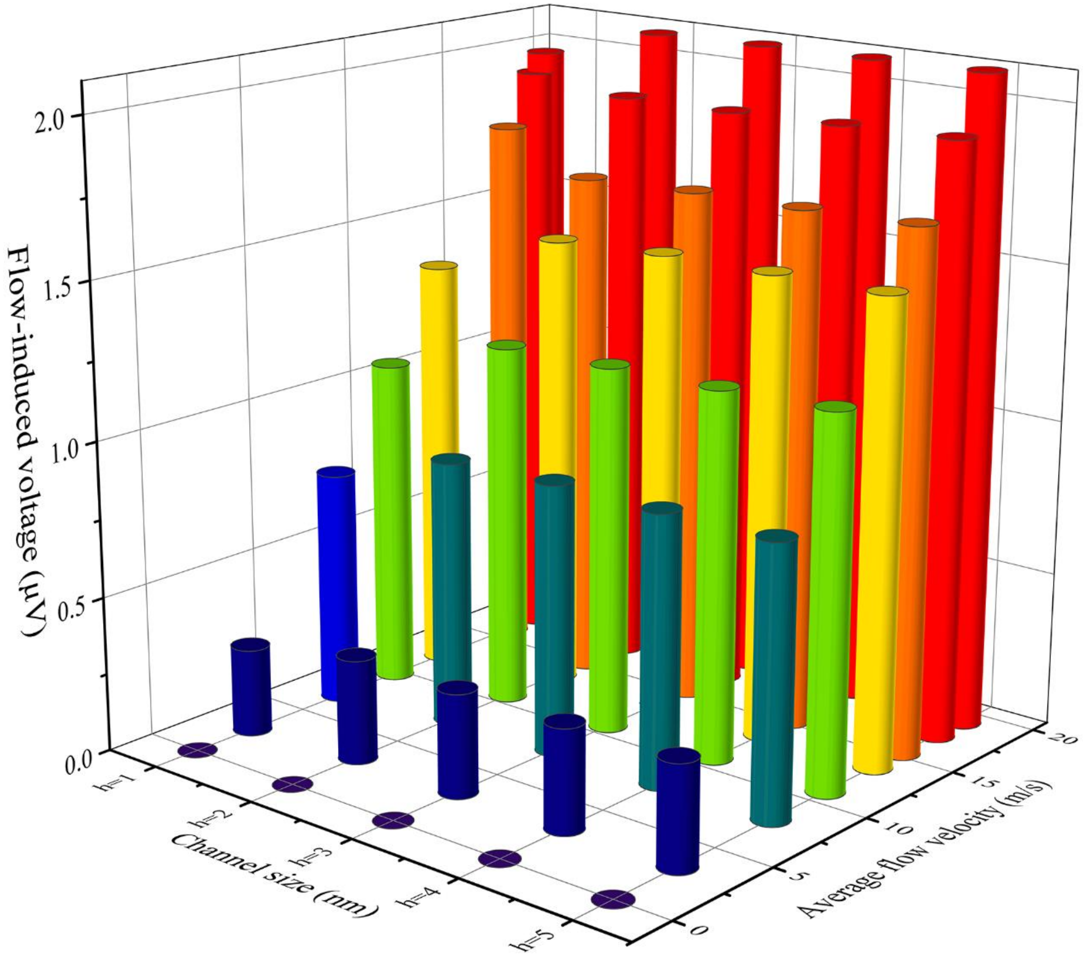
h = 1, 2, 3, 4, 5 nm

The average flow velocities of cations and anions increase as the graphene nano-channel size increases, eventually tending toward saturation.



Results and Discussion

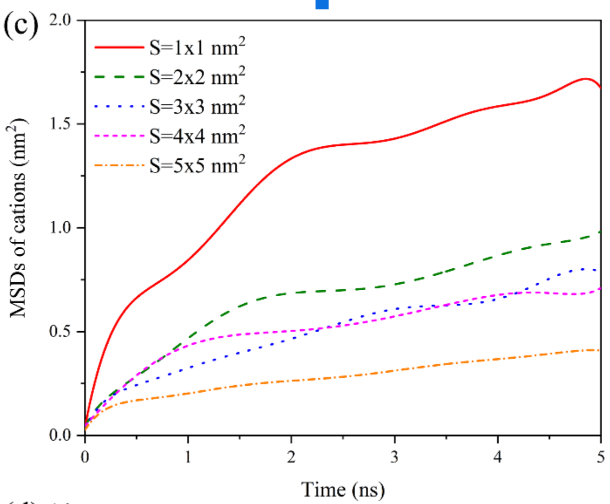
❖ Channel size effect

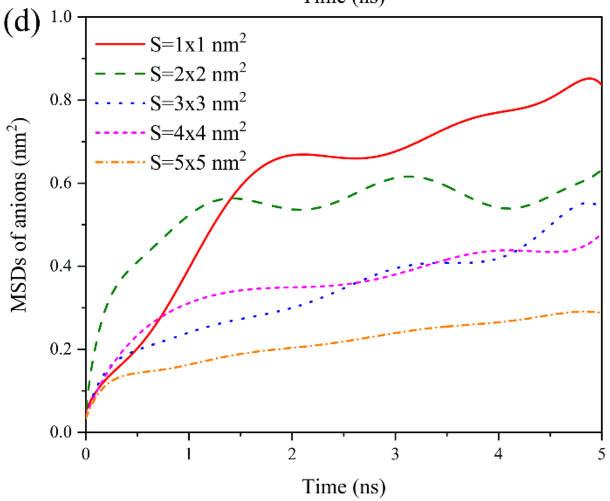


The flow-induced voltage increases from 1.9 to 2.1 μV as the graphene nano-channel size increases from 1 to 5 nm, tending toward saturation as average flow velocity increases.

Results and Discussion

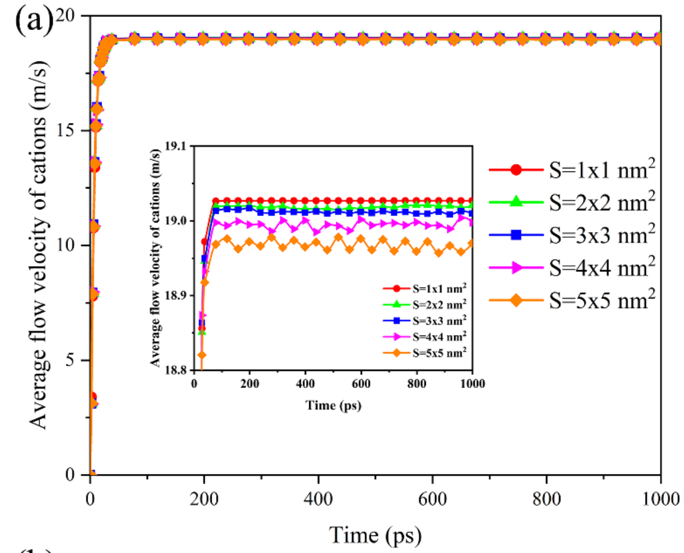
❖ Graphene area effect

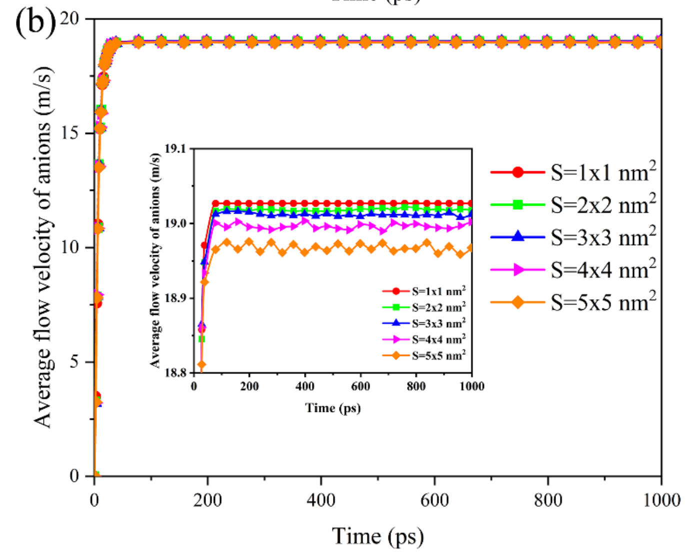




S = 1, 4, 9, 16, 25 nm²

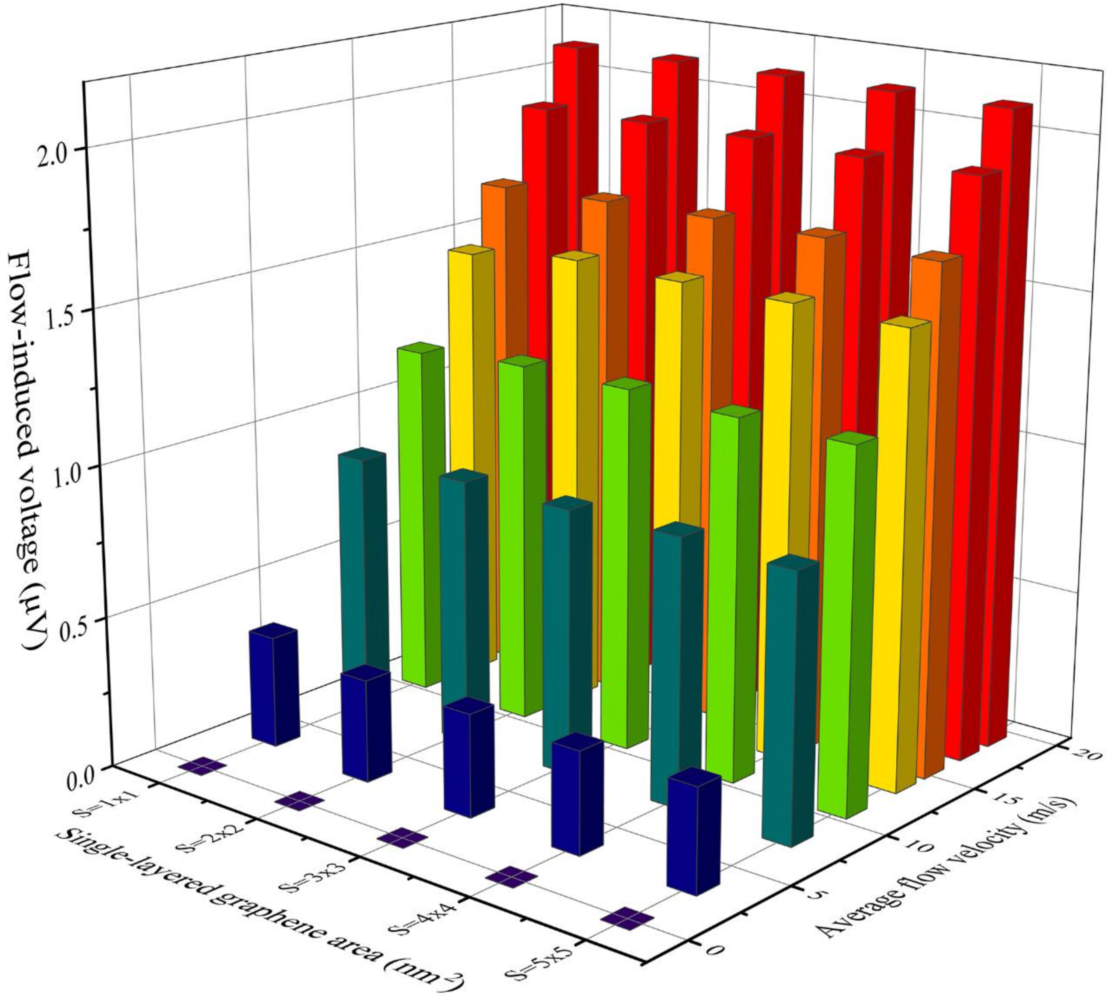
The average flow velocities of cations and anions increase as the graphene area decreases, eventually tending toward saturation.





Results and Discussion

❖ Graphene area effect



The flow-induced voltage decreases from 2.3 to 2.1 μV as the graphene area increases from 1 to 25 nm^2, then tending to saturation as average flow velocity increases.

Conclusions

- **Combing ILs and graphene channel to study the generation of flow-induced voltage using MD simulation**
- **Developing an advanced equation to calculate the flow-induced voltage on the nano-scale**
- **The flow-induced voltages increase from 2.1 to 2.4 μV as temperature increases from 300 to 375 K**
- **The flow-induced voltages increase from 1.9 to 2.1 μV or decrease from 2.3 to 2.1 μV as channel size or graphene area increase from 1 to 5 nm or from 1 to 25 nm^2**

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Thank you for your attention !

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