Flow-induced Voltage Generation by Driving Imidazolium-Based Ionic Liquids over a Graphene Nano-Channel

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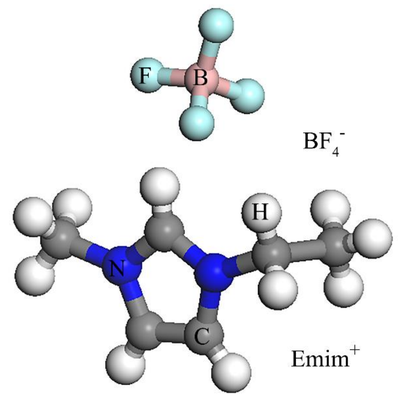
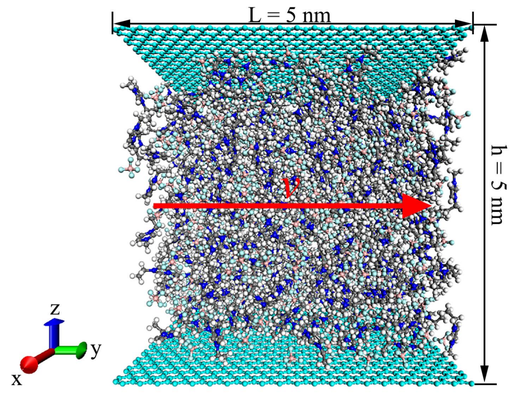
Introduction

Room temperature ionic liquids (RTILs) are novel soft functional materials, the physicochemical properties of RTILs can be easily manipulated by tuning the functionalization or the combination of the cations and anions for task-specific applications. Molecular dynamics (MD) simulation is a powerful tool to understand molecular or atomic details and has been widely employed to study the nanofluids. Herein, we employed MD simulation to investigate the generation of flow-induced voltage through driving ILs over graphene nano-channel. The flow-induced voltage can be potentially applied in nanoelectromechanical systems and offer much promise for bio-molecular sensing and bio-medical fields.

Model & Methods





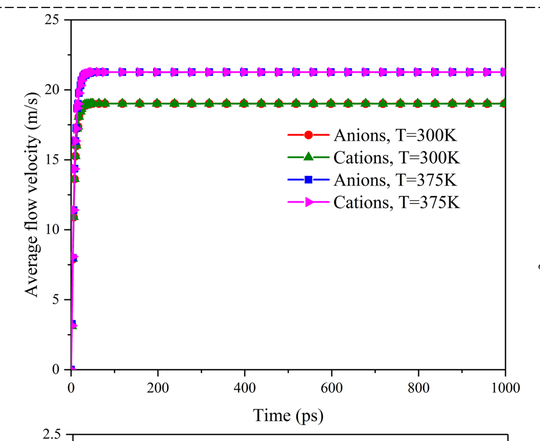
The simulated model is comprised of 1-ethyl-3-methylimidazolium tetrafluoroborate ([Emim][BF_4]) ILs and graphene channel. After the simulated systems reach equilibration, a series of accelerations from 0.001 to 0.2 nm ps^{-2} are applied in systems along y direction.

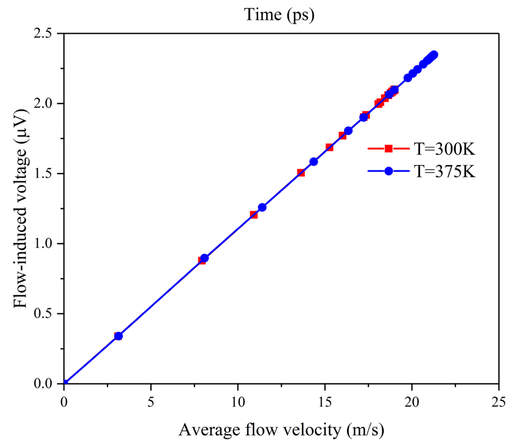
Calculated Equation

Considering the combined effect of cations and anions in the adsorbed layer on the free charge carrier of the graphene surfaces and the characteristic of Coulomb's law, we develop an advanced equation which can effectively and accurately calculate the flow-induced voltage of ILs and graphene nano-channel system on the nano-scale.

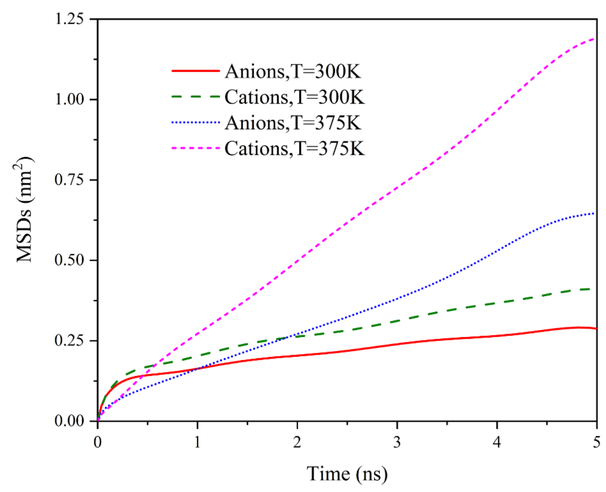
$$V = R\sigma eL\left(v^{+} - \frac{\left|\int_a^b \frac{1}{z^2}\rho^{-}(z)\,dz\right|}{\left|\int_a^b \frac{1}{z^2}\rho^{+}(z)\,dz\right|}v^{-}\right)$$

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



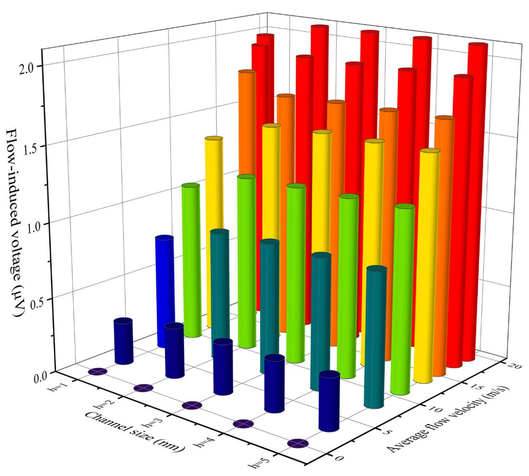


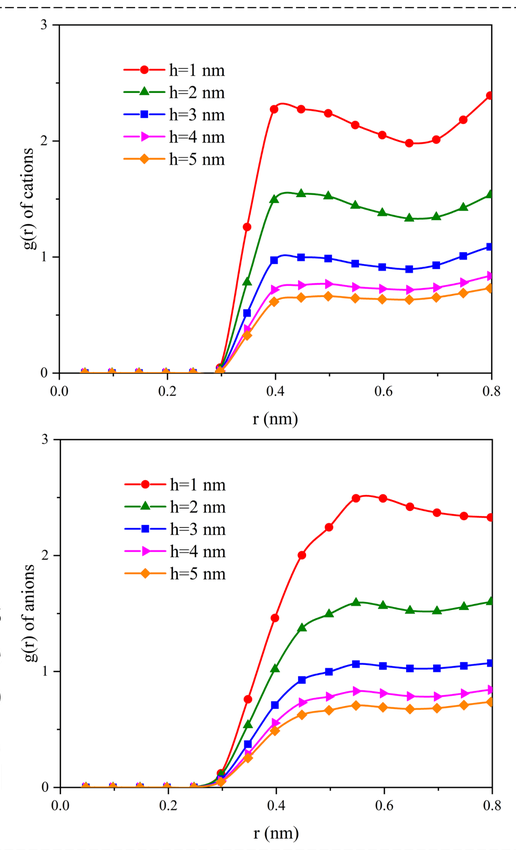
Temperature



The flow-induced voltage (2.4 μV) has a significant increase at T = 375 K which could be attributed by the change of viscosity (mean square displacements).

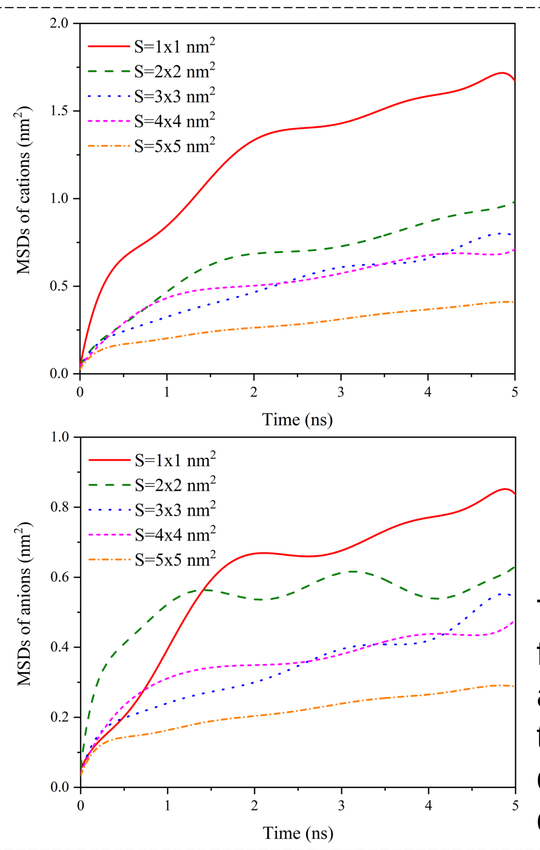
Channel Size

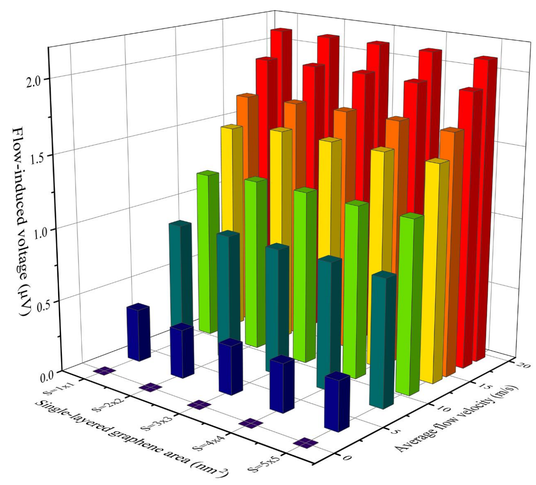




The flow-induced voltage increases from 1.9 to 2.1 μV as the graphene nano-channel size increases from 1 to 5 nm and then tends to saturation, which is quantified by the radial distribution function of ions.

Graphene Area





The flow-induced voltage decreases from 2.3 to 2.1 μV as the graphene area increases from 1 to 25 nm^2 and then tends to saturation, which is quantified by the mean square displacements of cations and anions.

Conclusions

In this work, the model consisting of ILs and graphene nano-channel is employed to investigate the generation of flow-induced voltage. An advanced equation is developed to effectively and accurately calculate the flow-induced voltage on the nano-scale. According to our developed advanced equation, we find that the flow-induced voltages increase from 2.1 to 2.4 μV as temperature increases from 300 to 375 K and increase from 1.9 to 2.1 μV or decrease from 2.3 to 2.1 μV as channel size or graphene area increases from 1 to 5 nm or from 1 to 25 nm^2.

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