# Asymmetry mechanism of anion and cation transporting in angstrom-scale graphene channels

***YanZi Yu[1], HengAn Wu[1], and †FengChao Wang[1]**

[1] CAS Key Laboratory of Mechanical Behavior and Design of Materials, Department of Modern Mechanics, University of Science and Technology of China, Hefei, Anhui 230027, China.

*Presenting author: yuyz@mail.ustc.edu.cn
†Corresponding author: wangfc@ustc.edu.cn

## Abstract

Ions transporting in narrow graphene channels is a rapidly growing research field because of its high transporting efficiency and low energy cost, with promise for many applications, such as nanofiltration, water desalination, energy harvesting and storage. Actually, the dimensions of the capillaries are crucial for ion transport, in especial the dimensions approach the size of small ions and water molecules. That's because the diameters of hydrated ions play a significant role as ions transporting in graphene capillaries. In this work, we focus on the charge asymmetry mechanism of $K^+$ and $Cl^-$ transporting in angstrom-scale graphene channels. Both ions share the similar mobility in bulk condition, whereas it reduced with different degrees in angstrom-scale confinement. The mobility of $Cl^-$ decreased more sharply than $K^+$. As ions transporting in the channels, the first hydration layer acted as the main factor to dominate their dynamical properties. What's more, the different water dipolar orientations of anion and cation leaded to different tribological behavior, and the oxygen-hydrogen bond in the first hydration layer of $Cl^-$ preferentially pointed to graphene wall more closely than that of $K^+$ with hydrogen approaching to graphene surface. Hence, the $Cl^-$ experienced a larger friction and smaller mobility than $K^+$. These understandings are integrated into a picture to understand transporting mechanism of anion and cation in graphene channel, and provide a reference for the rational design of functional membranes for daily applications.

Keywords: **Ion transport, Graphene channel, Angstrom-scale, Charge asymmetry**