Electronic Supplementary Information

The confined [Bmim][BF_4] ionic liquid flow through graphene oxide nanochannel: A molecular dynamics study

Yanlei Wang, Feng Huo, Hongyan He, and Suojiang Zhang**

Beijing Key Laboratory of Ionic Liquids Clean Process, CAS Key Laboratory of Green Process and Engineering, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

*Corresponding Author.

Tel: +86-10-82544875 E-mail: hyhe@ipe.ac.cn

Tel: +86-10-82544875 E-mail: sjzhang@ipe.ac.cn

Supplementary Figures and Captions:

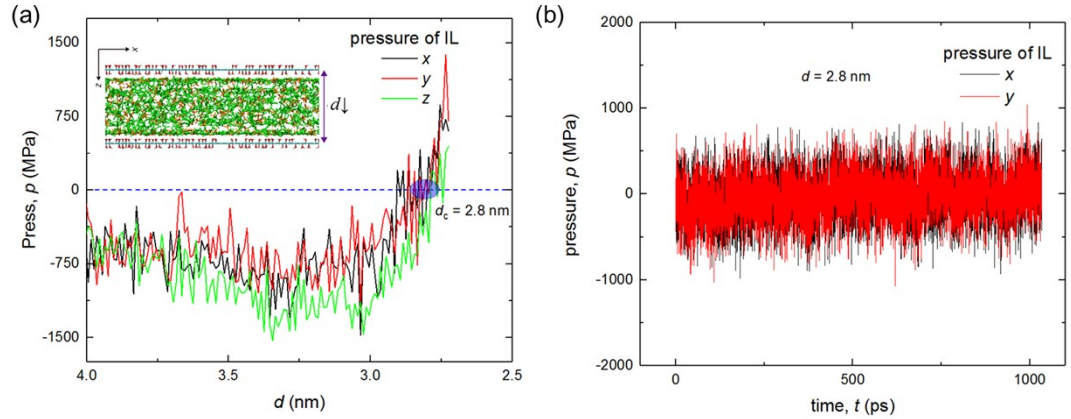


Figure S1. (a) The pressure-distance relations when decreasing the interlayer distance d in the MD simulations, showing a critical distance d_c = 2.8 nm, and the pressure is calculated via

$$p_{xx} = \frac{1}{V}\sum_{i=1}^{N}[m_i v_x^2 + \frac{1}{2}\sum_{n=1}^{N_{pair}}\sum_{j=1,2} r_{i,jx}F_{i,jx} + \frac{1}{2}\sum_{n=1}^{N_b}\sum_{j=1,2} r_{i,jx}F_{i,jx} + \frac{1}{3}\sum_{n=1}^{N_{ang}}\sum_{j=1,2,3} r_{i,jx}F_{i,jx} + \frac{1}{4}\sum_{n=1}^{N_{dih}}\sum_{j=1,2,3,4} r_{i,jx}F_{i,jx} + \text{Kspace}(r_{i,x}, F_{i,x})]$$

where N, N_{pair}, N_b, N_{ang} and N_{dih} are the number of atom, atom pairs, bonds, angles, dihedral angles in the system, r is the position of the specific atom, and F is the force on the specific atom resulting from the pairwise interaction. When d is larger than the critical distance, the pressure of the system will be a negative one. The negative pressure in the simulation originates from the mathematic calculations and is just a "nominal pressure" of the system. (b) The pressure of IL in the nanochannel with d = 2.8 nm as a function of the simulation time, indicating a zero pressure along x and y directions.

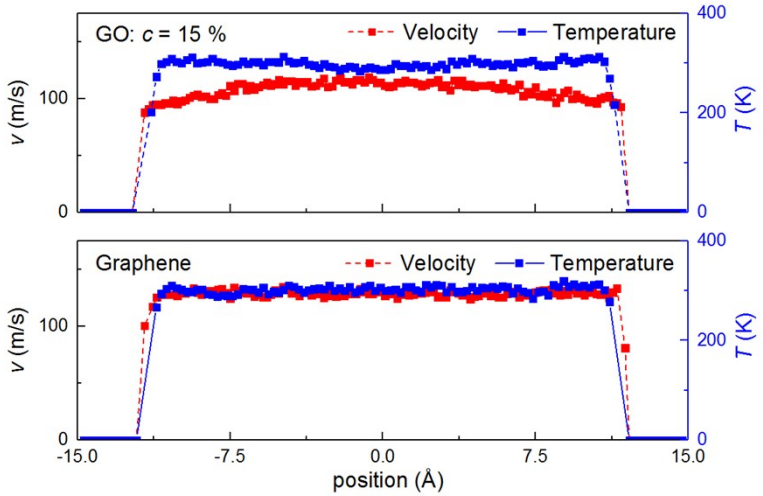


Figure S2. The distribution of temperature and velocity of the IL flow in nanochannel of graphene and GO with c = 15%, where temperature is calculated through the kinetic energy that subtracting out the spatially-averaged center-of-mass velocity field.

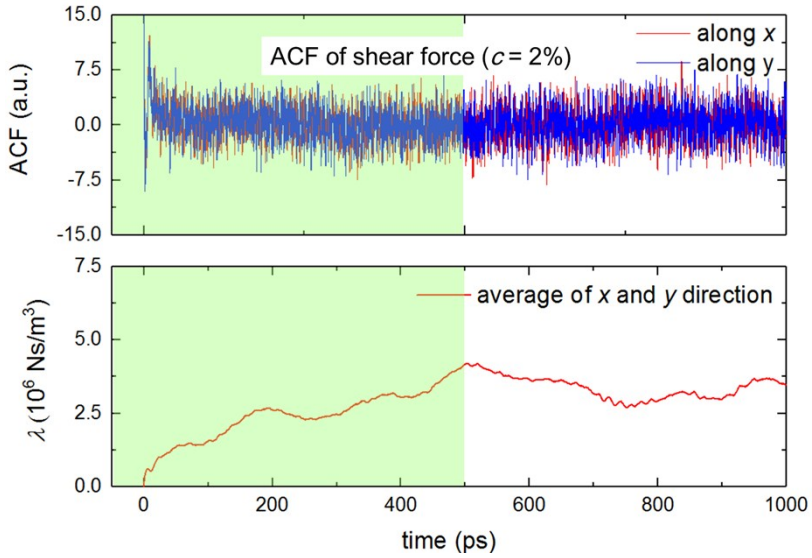


Figure S3. The autocorrelation function (ACF) of shear force and the integral friction coefficient of IL in GO with c = 2%, indicating that the friction coefficient will up to convergence at ~500 ps.

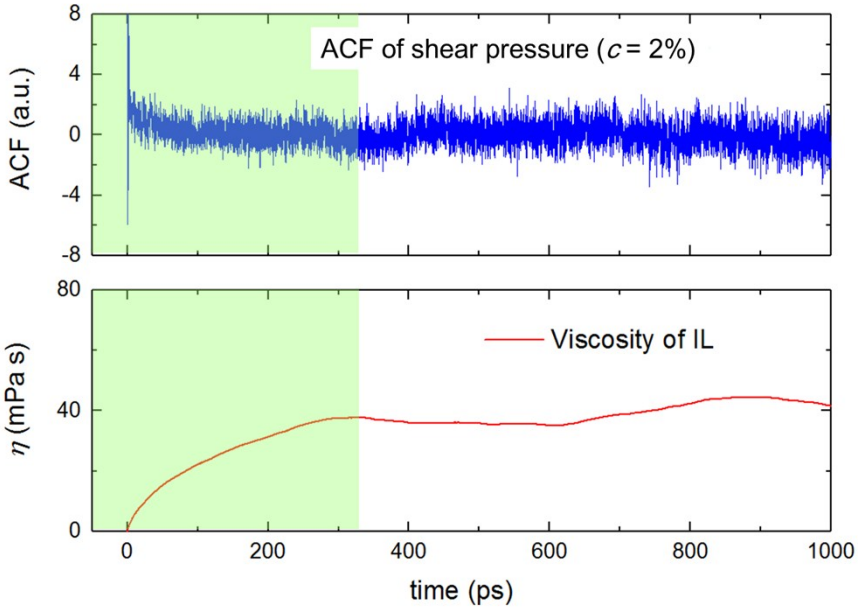


Figure S4. The autocorrelation function (ACF) of shear pressure and the integral viscosity of IL in GO with c = 2%, indicating that the viscosity will up to convergence at ~300 ps.

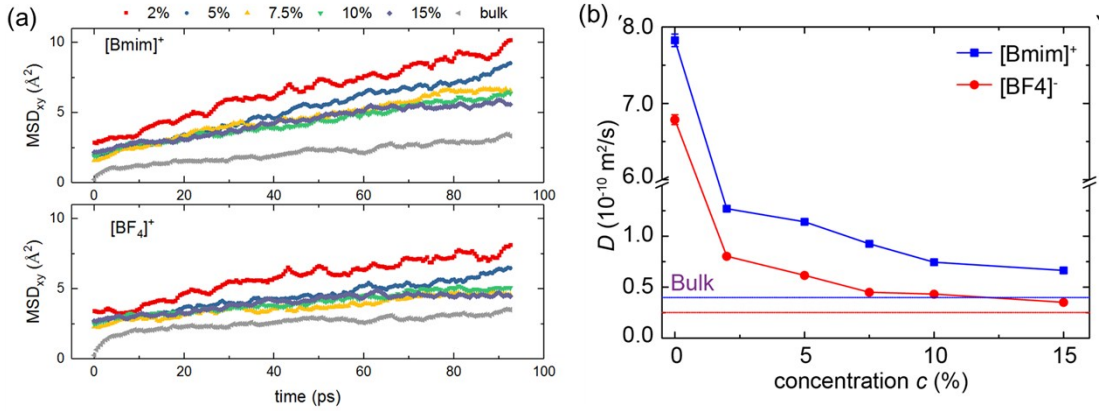
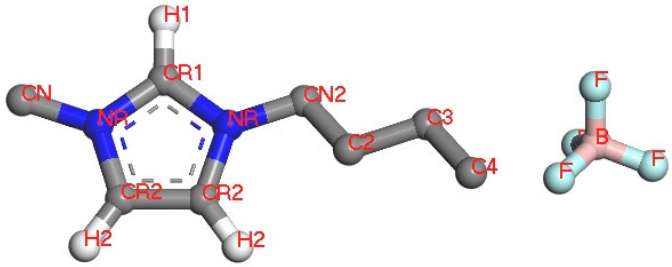


Figure S5. (a) Mean-square distance (MSD) of cation and anion in x and y plane, calculated in GO nanochannel with different concentration of hydroxyls. (b) Diffuse coefficient D_{xy} of cations and anions in the *xy* direction as a function of the concentration, where D is calculated via the equation, $D = \lim_{t\to max} <|\mathbf{r}(t) - \mathbf{r}(0)|^2>/2d_i t$. Here, d_i is the dimension of space, t is the simulation time, and <…> is the ensemble average.

Table S1 The partial charge of atoms in GO (*J. Am. Chem. Soc.* 1996, 118, 11225)

Atom type	Charge (*e*)
H	0.3294
O	-0.5260
C1 (connected to -OH)	0.1996
C2(non-hydroxylated carbon)	0.0000

Table S2 The partial charge of atoms in IL (*J. Phys. Chem. B*, 2010, 114, 4572)



Atom type (Bmim)	Charge (*e*)	Atom type (BF_4)	Charge (*e*)
NR	0.015	B	0.428
CR1	0.000	F	-0.307
H1	0.150		
CR2	-0.160		
H2	0.200		
CN	0.260		
CN2	0.230		
C2	0.050		
C3	0.000		
C4	0.000		