

Supplementary Material
**Nano- and macroscale study of the lubrication of titania using
pure and diluted ionic liquids**
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Macrotribology

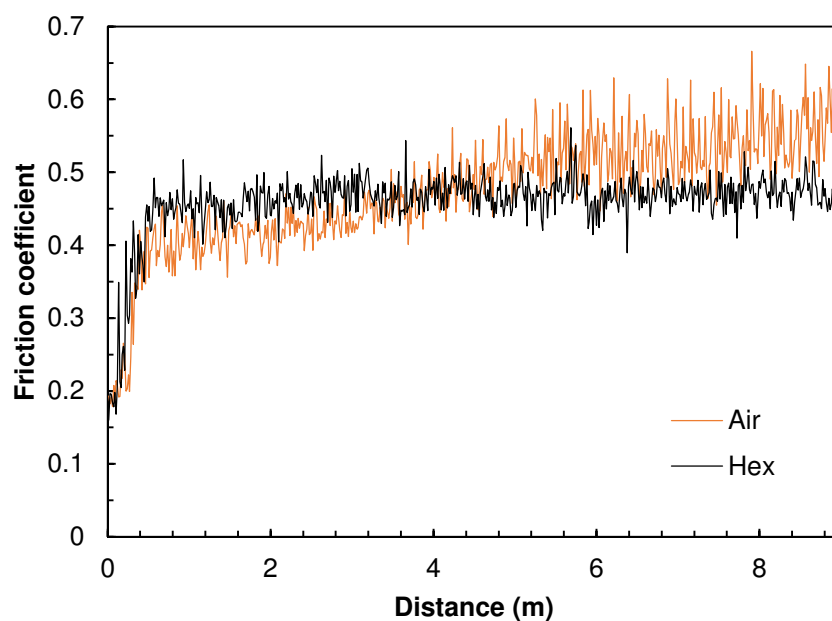


FIGURE S1 | Friction coefficient vs sliding distance measured in air and hexadecane under a load of 5 N and at 25 °C.

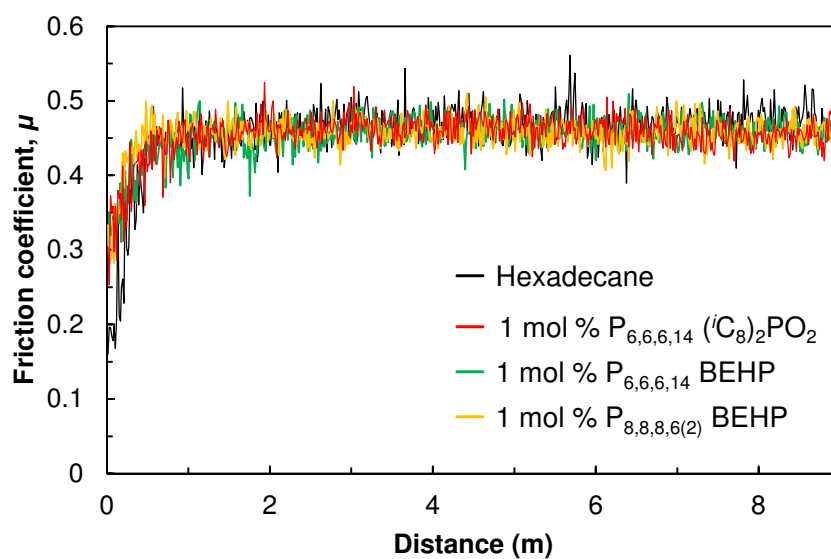


FIGURE S2 | Friction coefficient as a function of sliding distance for three stainless steel balls sliding on a titanium surface in 1 mol % mixtures of IL in hexadecane. Sliding was carried out under 5 N of normal load and a temperature of 25 °C.

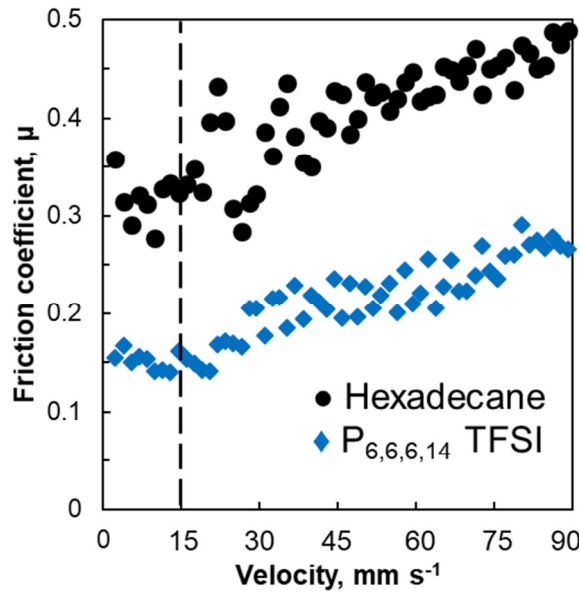


FIGURE S3 | Friction coefficient as a function of velocity for three stainless steel balls sliding on a titanium surface in hexadecane (black circles) and P_{6,6,6,14} TFSI (blue diamonds). The dashed line shows the velocity at which the other experiments were carried out. Sliding was carried out under 5 N of normal load and a temperature of 60 °C.

Calculation of Hertzian Contact Stress

The effective Young's modulus E_w can be calculated by:

$$\frac{1}{E_w} = \frac{1}{2} \left(\frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \right)$$

Where E_1 , E_2 are the elastic moduli and ν_1 , ν_2 are the Poisson's ratios associated with each body.

Contact area radius is given by:

$$a \cong \left(\frac{3RF}{2E_w} \right)^{1/3}$$

Where R is the radius of the sphere. F is the applied load.

Contact stress:

$$p_{max} = \frac{3F}{2\pi a^2}$$

The parameters used:

Titania: $E = 230$ GPa, $\nu = 0.28$

Stainless Steel: $E = 200$ GPa, $\nu = 0.3$

Macrotribology test:

$$F = 5 \text{ N}, p_{max} = 0.5 \text{ GPa}$$

$$F = 10 \text{ nN}, p_{max} = 0.6 \text{ GPa}$$

In the nanotribology tests the exact dimensions and geometry of the tip are uncertain and subject to change. The contact pressures are significantly higher:

$$F = 50 \text{ nN}, p_{max} = 11.8 \text{ GPa}$$

$$F = 200 \text{ nN}, p_{max} = 18.7 \text{ GPa}$$

Hamrock and Dowson model

Using the Hamrock and Dowson model the central film thickness, h_c , can be calculated by the following equation (Stachowiak and Batchelor, 2005):

$$\frac{h_c}{R'} = 2.69 \left(\frac{U\eta_0}{E'R'} \right)^{0.67} (\alpha E')^{0.53} \left(\frac{W}{E'R'^2} \right)^{-0.067} (1 - 0.61e^{-0.73k})$$

where a is the contact area radius from eq(2), U is the sliding velocity, η_0 is the viscosity of the lubricant at ambient pressure, E_w is the effective Young's modulus from eq(1), α is the pressure-viscosity coefficient, F is the applied load, and k is the ellipticity parameter. $k = 1$ for point contact. The pressure – viscosity coefficient of hexadecane varies from 11.6 to 13.2, and average of 12.5 is used here (Pensado et al., 2008; Paredes et al., 2012). For the pure ILs used in this study, the pressure-viscosity coefficient was not found in the literature. According to previous studies, the pressure-viscosity coefficient of ILs are generally between 12~21 GPa^{-1} (Pensado et al., 2008; Paredes et al., 2012; Mordukhovich et al., 2013; Gaciño et al., 2015), thus here the film thicknesses of the systems are calculated by assuming the limit values of 12 GPa^{-1} and 21 GPa^{-1} for the pure ILs.

Table S1 shows the calculated film thicknesses do not vary significantly for different chosen values of the pressure-viscosity coefficient.

TABLE S1 | The pressure-viscosity coefficients and calculated film thicknesses h_c for the lubricants used in this study.

Lubricant	h_c (nm)		h_c (nm)	
	$(\alpha = 12 \text{ GPa}^{-1})$		$(\alpha = 21 \text{ GPa}^{-1})$	
	5 N	10 N	5 N	10 N
P _{6,6,6,14} TFSI	18	18	25	24
P _{8,8,8,6(2)} BEHP	55	52	74	70
P _{6,6,6,14} BEHP	40	39	54	52
P _{6,6,6,14} (<i>i</i> C ₈) ₂ PO ₂	42	40	56	54
Hexadecane	1	1	1	1

References

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