Lateral Ordering in Nanoscale Ionic Liquid Films Between Charged Surfaces Enhances Lubricity

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Friction is responsible for significant energy losses on the industrial scale as well as for material fatigue, degradation and mechanical failure. Therefore, the ability to tune friction is extremely important in many research fields such as biomedicine, engineering, chemistry, physics, and nanotechnology [1]. Introducing a thin nanometric liquid film between the sliding surfaces at nanometer distance, can significantly reduce friction losses and the material wear in nanodevices. Room Temperature Ionic liquids (RTILs) are promising lubricants because of their unique thermophysical properties: chemical and thermal stability, low vapour pressure and low melting temperature [2]. Furthermore, electric field have been used to modify the structural and dynamic properties of RTILs, opening new avenues to develop tunable lubrication devices [3–6].

We systematically investigate the impact of RTIL composition and molecular structure on friction, by using gran canonical non–equilibrium molecular dynamics [3, 7]. Using both coarse grained and atomistic models of 1–*n*,2–methyl–imidazolium tetrafluoroborate [$C_{n=2..6}$MIM][BF_4] RTILs, we show that the friction force depends significantly on the chain length of cation and the surface charge [7]. RTILs composed of short cations are less compressible and show lower friction force. When the nanofilm is under high pressure, the friction force changes slope when increasing the surface charge, featuring a maximum where the slippage plane moves from the RTIL-electrode interface to the interior of the film.

We extend our analysis considering imidazolium cations and widely used anions, featuring different molecular structures, spherical (BF_4), elongated surfactant--like (C_2SO_4) and elongated with a more delocalized charge (NTf_2) [8]. Our results show that surface charge and anion geometry favours the crystallization of BF_4, and NTf_2 nanofilms, resulting in friction forces lower than the ones obtained for C_2SO_4 which forms disordered layers. We identify the formation of crystal–like structure as a new mechanism to tune the friction response with electric fields.

References

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