# Understanding the structure of ionic liquids on solid substrates by Atomic Force Microscopy experiments

Layla Bou Tannous[1,2], Mirella Simoes Santos[1], Zheng Gong[1], Agilio Padua[1], Audrey Steinberger[3]

[1] Laboratoire de Chimie, UMR 5182, Ecole Normale Supérieure de Lyon
[2] Leti, CEA, Université Grenoble Alpes
[3] Laboratoire de Physique, UMR 5672, Ecole Normale Supérieure de Lyon

Ionic liquids are molten salts at ambient temperature, which are increasingly used as high-performance solvents, lubricants and electrolytes. The way they organize at the molecular level on solid substrates is crucial in many applications. In heterogeneous catalysis and electrochemical sensing, it impacts the selectivity and the efficiency of the process. In lubrication, it governs the wear efficiency and the friction coefficient. It also affects the maximal energy density and lifetime of energy storage devices, and controls the conductivity of semiconducting nanosheets and nanowires in novel electronic devices. However, the interfacial structure of ionic liquids remains challenging to understand.

We have developed force spectroscopy experiments using an Atomic Force Microscope (AFM), where the interaction force between the substrate and a probe in the ionic liquid medium is measured as a function of the probe-substrate distance z. Using this technique, we have characterized the organization of an ionic liquid (1-octyl-3-methylimidazolium dicyanamide: $C_8$mimDCA) on various substrates, and obtained an excellent agreement with molecular dynamics (MD) simulations as shown in figure 1. Our results have already enabled us to rationalize the effect of the surface chemistry on the interfacial structure of a long chain imidazolium-based ionic liquid [1]. Our AFM expertise can be further used to benchmark MD simulations, or explore systems that are too complex to be simulated yet.

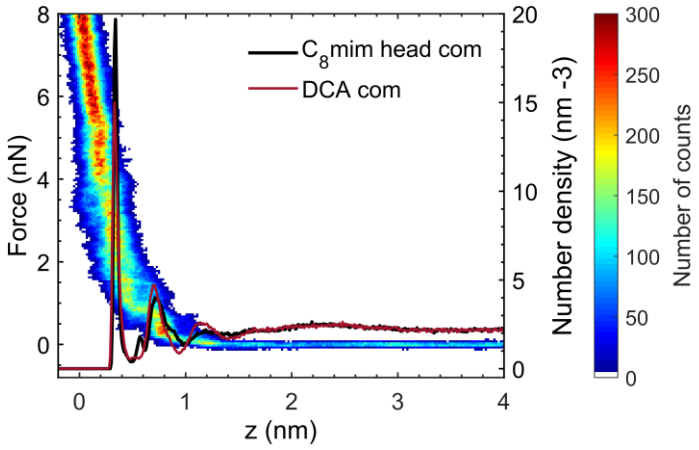


**Figure 1** AFM 2D force versus distance z histogram in $C_8$mimDCA on molybdenum disulfide, generated from 10 individual approach curves. Density profiles of the center of mass of the imidazolium head of the $C_8$mim cation and of the DCA anion, obtained by MD simulations, are superposed on the experimental results. From [1].

**References :**

[1] L. Bou Tannous, M. Simoes Santos, Z. Gong, P.-H. Haumesser, A. Benayad, A. A. H. Padua, A. Steinberger, Langmuir 39 (2023) 16785-16796.

**Mots clés : Ionic liquids, Interfacial structure, Atomic Force Microscopy, Force spectroscopy**