

Understanding the Structure of Ionic Liquids on Solid Substrates: Towards a More Sustainable Ammonia Production

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Location: Laboratoire de Physique, ENS de Lyon, 69007 Lyon, France

Calendar: M2 internship: 4 to 6 months between Jan. 2024 and Aug. 2024 (remunerated)
PhD thesis: 3 years starting Sept. or Oct. 2024, funding by application at ED PHAST

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Ionic liquids are molten salts at ambient temperature, which are increasingly used as 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, as it depends on the chemistry of the ionic liquid, on the nature and topography of the substrate, and on other parameters such as the bulk water content of the ionic liquid. **It can be characterized experimentally by 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, as shown in Figure 1(a). When the probe-substrate distance is reduced, a force increase followed by an abrupt change of slope is the signature of the compression of the interfacial structure followed by a reorganisation.

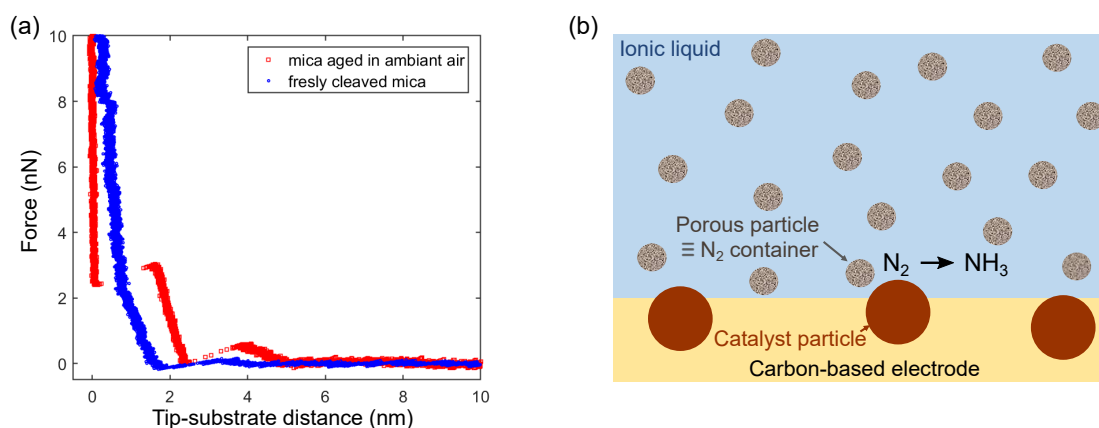


Figure 1: (a) Force as a function of the distance between the AFM tip and the mica surface in the ionic liquid 1-decyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide, for mica aged 1h in ambient air (red squares) and freshly cleaved mica (blue circles). Unpublished data acquired by Layla Bou Tannous during her PhD. (b) Schematic representation of the GREENH3 project for a sustainable ammonia production.

In the M2 internship or PLR, we will use AFM measurements to investigate open questions on the organization of ionic liquids on mica, which is a key reference substrate in force spectroscopy techniques (Surface Force Apparatus and AFM). We will build upon the experimental work of Layla Bou Tannous, who defended her PhD in April 2023. She noticed that the interfacial structure of an ionic liquid depended strongly on the handling of the mica substrate prior to its immersion in the ionic liquid (Figure 1(a)). We have also gathered clues that the ionic liquid structure may present lateral heterogeneities on mica, which is both unexpected and intriguing. The aim of this internship is to complete the preliminary experiments initiated by Layla Bou Tannous on mica in order to publish these results, and to develop cartography tools to investigate the structure of the ionic liquid over a wide surface.

The proposed PhD project focuses on systems of interest for an energy transition challenge: ammonia is a promising zero-carbon fuel, but the current industrial process for ammonia production is too energy-intensive. Indeed, it already consumes about 1.5% of the world's production of energy for producing ammonia that is mainly used for the fabrication of fertilizers, refrigerants, and plastics, not as a fuel. The GREENH3 project, funded by the PEPR Hydrogène, aims at **developing a more sustainable process for ammonia production** from atmospheric nitrogen. It relies on novel catalyst nanoparticles embedded in a carbon-based electrode, working in an ionic liquid medium seeded with porous particles that act as nitrogen containers, as depicted in Figure 1(b). **We will investigate experimentally by AFM the various interfaces of interest for the GREENH3 project, in order to build an experimental understanding of the interfacial structure of the ionic liquid on the catalyst particles, which is important for the efficiency of the nitrogen reduction, and on the porous particles, which is important for the stability of the particle suspension.** Additionally, we will directly study the interaction between two porous particles and between a porous particle and the electrode, by grafting a porous particle on an AFM tip. The gathered knowledge will help select or design the best ionic liquid for this new catalytic process, and develop other ones.

Collaborators: Margarida Costa Gomes (Laboratoire de Chimie, ENS de Lyon, CNRS)
Agilio Padua (Laboratoire de Chimie, ENS de Lyon, CNRS)
Stephane Daniele (CP2M, CPE Lyon, Université Lyon 1, CNRS)

Application: If you are motivated by this interdisciplinary project at the crossroad of physics and chemistry that addresses an energy transition challenge, please contact Audrey Steinberger (audrey.steinberger@ens-lyon.fr) for additional scientific and practical details. In return, you will be asked to provide a written statement explaining your motivation for this project, a CV, and the contact information of one or two previous internship advisors.