

Ionic liquids as tuneable solvents for exfoliation of graphene

Emilie Bordes

Margarida Costa Gomes and Agilio Pádua

*Institut de Chimie de Clermont-Ferrand,
Université Clermont Auvergne, CNRS, 63000
Clermont-Ferrand, France*

Emilie.Bordes@univ-bpclermont.fr

Mass production and commercial availability are requirements for wider applications of graphene in electronic, electrochemical and optical fields. [1] The production graphene from graphite in a liquid-phase is one of the most promising ways to achieve large-scale production at low cost. The exfoliation process can be conceptually explained in three steps: intercalation of solvent between layers, dispersion of the 2D-material, and stabilization in the liquid-phase. The exfoliation mechanism is an important factor that needs deep understanding step by step and should provide useful information on how to efficiently achieve high-quality graphene by optimising the exfoliation process. Ionic liquids are molten salts with melting points below 100°C. They have a high chemical variety (See Figure 1.) with many cation-anion combinations that lead to tuneable physicochemical properties [2]. Ionic liquids have a number of potential advantages for the dissolution of carbon nanomaterials, such as their high ionic density, chemical and thermal stability, large electrochemical window and ease of recycling.

Our objective is to improve the current knowledge of the interactions involved between graphite and various chemical functions in order to find the best solvent capable of dissociating and stabilizing graphene layers. Samples of suspended graphene in different ionic liquids have been characterized in terms of

the size of the flakes, number of layers and total concentration. In order to rationalize our observations, via a thermodynamic approach, we have studied different polyaromatic compounds as models for the interactions of ionic liquids with graphene. The graphene – ionic liquid interfacial energy was evaluated through contact angle measurements. Molecular dynamics simulation of the exfoliation of one graphene layer from a stack of graphite provided a microscopic view of the intercalation of solvent molecules and of the energies involved. (see Figure 2.)

References

- [1] A. K. Geim and K. S. Novoselov, *Nat. Mater.*, **6**, (2007) 183–191.
- [2] T. Welton, *Chem. Rev.* **99** (1999) 2071-2083.

Figures

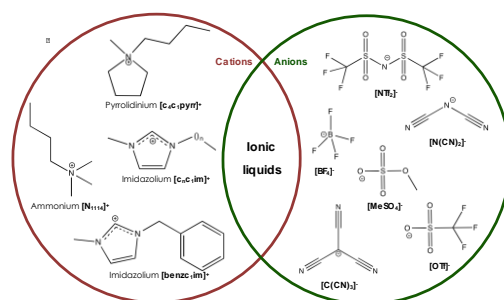


Figure 1: Examples of the chemical structures of the cations and anions, which constitute the ionic liquids studied.

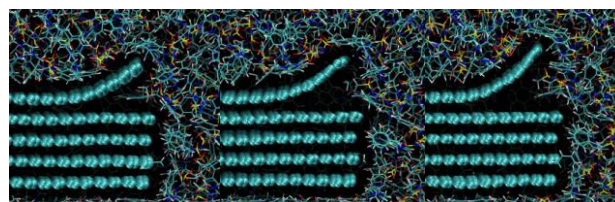


Figure 2: Ionic liquid surrounding a stack of five layers of graphene during a peeling experiment in molecular dynamics.