Exfoliation of graphene oxide using ionic liquids: experimental and molecular modelling approach

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Abstract

Graphene, a one-atom-thick planar sheet of sp^2 hybridized carbon, has received much attention due to its outstanding properties such as large specific surface area, high electrical and thermal conductivity, excellent chemical stability and mechanical stiffness. Graphite, which is cheap and readily available, consists of stacked graphene sheets. Therefore, one of the most convenient methods for the mass production of graphene sheets is the exfoliation of graphite in the liquid phase. Recently, many attempts to produce graphene sheets in large quantities via chemical reduction of exfoliated graphite oxide (GO) have been reported. During the oxidation process of graphite, the unique electronic properties of graphene dramatically degrade. The electrical conductivity of the graphene oxide sheets can be partially restored by the reduction step; however, this results in their irreversible agglomeration. Therefore, different strategies to disperse graphene sheets before or during reduction step have been used, including stabilization by various polymeric dispersants or surfactants and covalent/non-covalent functionalization [1].

In this context, ionic liquid (ILs) can be used for functionalization of graphene. They can adsorb on the graphene surface through the noncovalent interactions of anion and/or cation with graphene. ILs present several advantages such as enhanced ionic conductivity, thermal stability and excellent mechanical properties. The graphene modified with ILs are endowed with improved conductivity, excellent hydrophilicity and positive charged [2]. The repulsion between the resultant cation-charged GO sheets, the charge transfer between the ions and graphene and the high solubility of the grafted IL contribute to the exfoliation of graphite into graphene sheets and to prepare long-term stable graphene dispersions using ILs [3].

In this work, several ILs with different chemical structures have been synthesized and employed for the modification of graphite and graphite oxide in order to show the possible exfoliation of graphene layers in both materials. The graphite oxide employed for the study has been prepared by the Hummers method. The average interlayer spacing between the exfoliated graphene layers in graphite and graphite oxide has been measured by X-ray diffraction (XRD) (figure 1). Molecular dynamics simulations were also used to study the influence of ILs in the interlayer spacing (figure 2).

References

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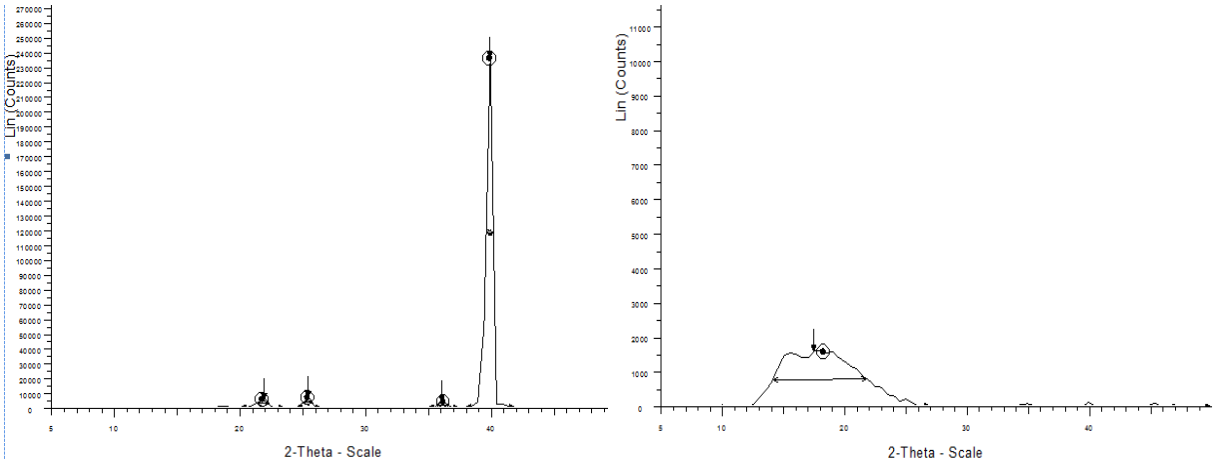
[2] R Marcilla, M Sánchez-Paniagua, B López-Ruiz, E López-Cabarcos, E Ochoteco, H Grande, D Mecerreyes, Journal of Polymer Science Part A: Polymer Chemistry, **44** (2006) 3958-3965.
[3] MH Ghatee, F Moosavi, Journal of Physical Chemistry C, **115** (2011) 5626-5636.

Figures



(a) (b)

Figure 1. XRD pattern of: a) graphite and b) graphite oxide.

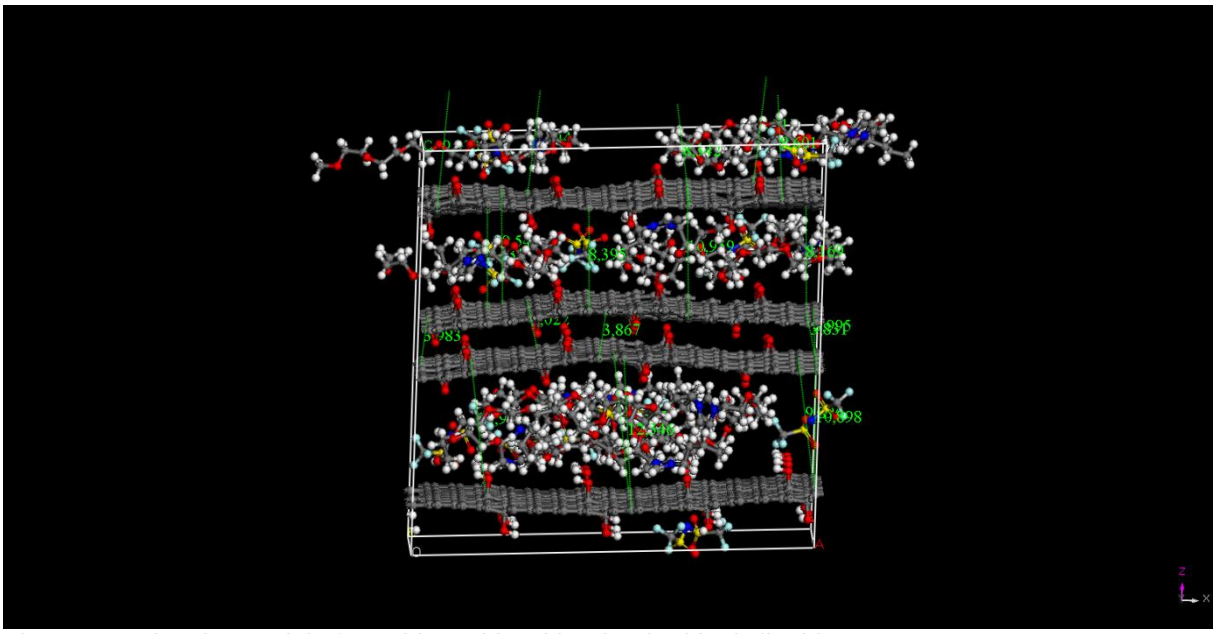


Figure 2. Molecular model of graphite oxide with adsorbed ionic liquid.