Evaluating the Surface Tension of Ionic Liquids Using the Langmuir Principle and Molecular Dynamics Structural Data

Karina Shimizu and José N. Canongia Lopes [C, S]
Centro de Química Estrutural, Instituto Superior Técnico, University of Lisbon, Lisbon, Portugal
jnlopes@tecnico.ulisboa.pt

Surface tension plays a crucial role in many of the operational problems faced by the chemical industry. In this context, an understanding of the nature of the interface between a liquid and a gas phase is of utmost importance. In this work, we address different issues related to the composition and structure of the surface layer of an ionic liquid under vacuum. Several efforts have been made to correlate in an empirical or semi-empirical way the surface tension of different ionic liquids with the characteristics of their constituting ions. Those works range from the use of quantitative structure-property relationship (QSPR) methods, to the definition of the so-called Parachor and Ionic Parachor (surface-tension-weighted molar volumes) and their use in group-contribution methods.[1-5] However, the complex structural nature of ILs requires considerable effort on the development of a general framework for explaining and predicting surface tension trends across a large number of different ILs.[6] Our approach uses the so-called Langmuir principle to correlate surface tension values along two different homologous series of ionic liquids. According to that principle, two matters are paramount to the correct evaluation and understanding from a molecular perspective of the surface tension: bulk cohesive energy and surface molecular orientation. The latter quantity is accessed via structural data obtained at the IL/vacuum interface using MD simulations.

References:

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